=> d ibib ab hitstr 1-41

L12 ANSWER 1 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER:
1398:660819 CAPLUS
COCUMENT NUMBER:
130:125266
TITLE:
Synthesis of a progesterone derivative and its
labeling with 1251
AUTHOR(S):
Huang, Wenlin, Lin, Meiling
Department of isotopes, China Institute of Atomic
Energy, Beijing, 102413, Peop. Rep. China
Tongweinu (1997), 10(4), 238-241
CODEN: TONGEN, ISSN: 1000-7512
YUBLISHER:
YUBLISHER:
YUBLISHER:
DOCUMENT TYPE:
JOURNAL
LANGUAGE:
AB Progesterone-11.alpha.-hemisuscinyl iodo-125-histamine [1251-PHH] can be
used for RIA. The synthesis of PHH and its labeling with 1251 was
described. The effect of the labeling conditions including the reaction
time, the amt. of PHH, the PH value of reaction buffer and the quantity of
chloramine-T on the labeling yield were studied. The labeling yield
reaches 733.
IT 219859-47-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of a progesterone deriv. and labeling with 1251)
RN 219859-47-9 CAPIUS
CN Pregn-4-ene-3,20-dione, 11-{4-[2-5-(iodo-1251)-1H-imidazol-4y1]ethyl]amino]-1,4-dioxobutoxy]-, (11.alpha.)- (9CI) (CA INDEX NAME)
Absolute stereochemistry.

Absolute stereochemistry.

L12 ANSWER 2 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN

PAGE 1-A PAGE 1-B

189894-04-OP
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(artificial cytochrome P 450 that hydroxylates unactivated carbons with regio- and stereoselectivity and useful catalytic turnovers)
18984-04-O CAPLUS
Androstane-3,17-diol, bis[4-(1,1-dimethylethyl)-.beta.-[2-oxo-2-[(2-sulfoethyl)]amino]ethyl]benzenepropanoate], (3.beta.,5.alpha.,17.beta.)(9CI) (CA INDEX NAME)

Absolute stereochemistry.

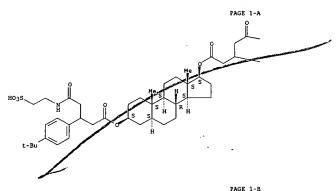
L12 ANSWER 2 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1997:672745 CAPLUS
DOCUMENT NUMBER: 127:356406
TITLE: An artificial cytochrome P450 that hydroxylates unactivated carbons with regio- and stereoselectivity and useful catalytic turnovers
AUTHOR(S): Breslow, Ronald; Huang, Ying; Zhang, Xiaojun; Yang, Jerry
CORPORATE SOURCE: Dep. Chem., Columbia Univ., New York, NY, 10027, USA
SOURCE: Dep. Chem., Columbia Univ., New York, NY, 10027, USA
CODEN: PNASA6; ISSN: 0027-8424
PUBLISHER: National Academy of Sciences of the United States of America (1997), 94(21), 11156-11159
COCUMENT TYPE: Journal
LANGUAGE: National Academy of Sciences
DOCUMENT TYPE: Journal
AB A catalyst has been synthesized comprising a manganese porphyrin carrying four beta-cyclodextrin groups. It catalyzes the hydroxylation of substrates of appropriate size carrying tert-butylphenyl groups that can hydrophobically bind into the cyclodextrin cavities. In one example as many as 650 catalytic turnovers are seen before the catalyst is oxidatively destroyed, and with a rate comparable to that of typical cytochrome P 450 enzymes. In another example, a steroid deriv. is regionand stereoselectively hydroxylated at a single unactivated carbon atom, but more slowly and with fever turnovers. The carbon attacked is not the most chem: reactive, and the selectivity is detd. by the geometry of the catalyst-substrate complex. Nonbinding substrates are not reactive under the conditions used, and substrates with more flexible binding geometries give more than a single product.

11 19256-58-6
RL: FMU (Pormation, unclassified); FORM (Formation, nonpreparative)
(artificial cytochrome P 450 that hydroxylates unactivated carbons with regio- and stereoselectivity and useful catalytic turnovers)

RN 19856-58-6 CAPIUS
N Androstane-3,6,17-triol, 3,17-bis[4-(1,1-dimethylethyl)-.beta.-[2-oxo-2-(2-yulfoethyl) amino] ethyl) benzenepropanoate],
(3.beta.,5.alpha.,6.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 2 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN



198560-57-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(artificial cytochrome P 450 that hydroxylates unactivated carbons with
regio- and stereoselectivity and useful catalytic turnovers)
198560-57-5 CAPLUS
Cholane-3, 24-diol, bis[4-(1,1-dimethylethyl)-.beta.-[2-oxo-2-{(2sulfoethyl)amino]ethyl]benzenepropanoate], (3.beta.,5.alpha.)- (9CI) (CA
INDEX NAME)

09/930,316 Page 3

L12 ANSWER 3 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN

L12 ANSWER 3 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1997.653283 CAPLUS
127:336532
L17:336532
AUTHOR(S): Effect of ionic strength on solution stability of PNU-67590A, a micellar producy of methylpredhisolone Okamoto, Hirokazu Mori, Kyokor Ohtsuka, Kumikor Ohuchi, Hiroyukir Ishil, Hiroaki
CORPORATE SOURCE: Pharmacia and Upjohn, Tsukuba Research Laboratories, Tsukuba, 300-42, Japan
Pharmaceutical Research (1997), 14(9), 1181-1185
CODEN: PHREEB; ISSN: 0724-8741
Plenum

SOURCE: Pharmaceutical Research (1997), 14(9), 1181-1185
CODEN: PHREEB, ISSN: 0724-8741
PUBLISHER: Plenum
DOCUMENT TYPE: Journal
LANGUAGE: English
AB PNU-67590A is a water-sol. micellar prodrug of methylprednisolone (MP).
The major products of degrdn. of PNU-67590A are MP by hydrolysis and methylprednisolone 17-suleptanate (17-E) by 21. Fwdarw.17 acyl migration. The effect of ionic strength on micelle formation and stability of PNU-67590A in aq. soln. was examd. PNU-67590A solns. at pH 2 and 8 and ionic strength of 0.05, 0.1, 0.2, and 0.4 M were maintained at 25.degree. C in the dark to measure MP and 17-E levels over time. The rate of degrdn. of micellar PNU-67590A at pH 8 was less than that of monomeric PNU-67590A, and vice versa at pH 2. Increase in ionic strength decreased both the crit. micelle concn. of PNU-67590A and the degrdn. of micelle PNU-67590A at both pHs, resulting in improved overall stability of PNU-67590A. Formulation of PNU-67590A in a concd. soln. with high ionic strength will maximize stability and shelf-life.

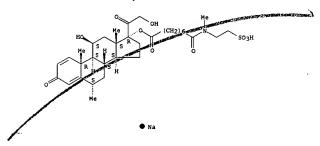
II 19776-67-3. Methylprednisolone 17-suleptanate
RI: PMU (formation, unclassified); FORM (formation, nonpreparative) (effect of ionic strength on soln. stability of PNU-67590A, micellar prodrug of methylprednisolone)
RN 197776-67-3 CAPLUS

RN 197776-67-3 CAPLUS

RN 2978-67-3 CAPLUS

Absolute stereochemistry.

Absolute stereochemistry.



L12 ANSWER 4 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1997:342359 CAPLUS
DOCUMENT NUMBER: 126:340291
TITLE: Selective Catalytic Hydroxylation of a Steroid by an Artificial Cytochrome P-450 Enzyme
Breslow, Ronald Z hang, Xiaojun; Huang, Ying
Department of Chemistry, Columbia University, New
York, NY, 10027, USA
Journal of the American Chemical Society (1997),
119(19), 4535-4536
CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society
Journal
LANGUAGE: English
AB A manganese-porphyrin carrying four cyclodextrin binding groups catalyzes
the hydroxylation of an androstane deriv. that can bind into two
cyclodextrin rings in water with catalytic turnover, and specific
hydroxylation at C-6 of the steroid. A dihydroxtilbene deriv. is also
catalytically hydroxylated by this catalyst system. Analogs of the
substrates that cannot bind into the cyclodextrin groups are unchanged
under the reaction conditions. A steroid with less specific binding is
also hydroxylated, but with a more random product pattern. This
artificial enzyme mimics cytochrome P 450 in its ability to bind a
substrate with selectivity and then hydroxylate a substrate position that
is not particularly reactive except for its geometric proximity to the
oxo-metal intermediate in the catalyst. Catalytic turnover is modest (4
to 14) since the catalyst is also oxidatively destroyed, but other work
indicates how such problems can be overcome to produce a high turnover
catalyst. Control reactions support the proposed mechanism.

IT 18384-04-0 18984-04-10
(RPC (Process)
(Biological study); PROC (Process)
(Biological study); PROC (Process)
(Selective catalytic hydroxylation of a steroid by artificial
cytochrome P 450 enzyme)

N 18384-04-0 CAPIUS

N Androstane-3,17-diol, bis (4-(1,1-dimethylethyl)-.beta.-[2-oxo-2-[(2sulfoethyl) aminol ethyl]benzenepropanoate], (3.beta.,5.alpha.,17.beta.)-

(Continued)

(Continued)

L12 ANSWER 4 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN

189894-05-1 CAPLUS Androstane-3,17-dio1, bis[5-oxo-5-[(2-sulfoethyl)amino]pentanoate], (3.beta.,5.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

(Continued)

Absolute stereochemistry.

PAGE 1-A (CH2) 3 PAGE 1-B

L12 ANSWER 5 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN

L12 ANSWER 4 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN

KIND · DATE APPLICATION NO. DATE

PATENT NO. KIND DATE

US 5622944 A 19970422 US 1995-434892 19950504
US 5607691 A 19970304 US 1995-449188 19950524
PRIORITY APPLN. INFO.:
US 1993-9463 19930127
US 1993-77296 19930614
US 1993-77296 19930614
US 1993-164293 19931209

OTHER SOURCE(S):

MARPAT 126:347221
AB Compns. and methods are provided for enhanced transdermal electrotransport of 17-hydroxy sterol compds., including testosterone. The parent sterols are modified at the 17-hydroxy position by covalent attachment of a charged chem. modifier. The chem. modifier provides the parent sterol with enhanced transport properties and is hydrolyzed under physiol. conditions to release the active parent compd. The compn. comprises a 17-hydroxy sterol/chem. modifier complex, more generally represented by the formula (sterol-0-)c(O)-R-N(R1) (R2) (R3)+, where N(R1) (R2) (R3)+ represents a quaternary amonium group and R1, R2, and R3 are independently selected from the group consisting of lower alkyl, alkyl, aryl, arylalkyl, cyclolkyl, heteroalkyl, and heteroarylakyl, or R1 and R2 together with the nitrogen to which they are attached form a substituted heterocycle and R3 is lower alkyl, and R is a linking moiety, linking the (sterol-0)-C(O)- to the nitrogen to which they are attached form a substituted heterocycle and R3 is lower alkyl, and R is a linking moiety, linking the (sterol-0)-C(O)- to the nitrogen atom.

IT 19803-21-5P

RL: ADV (Adverse effect, including toxicity); SPN (Synthetic preparation), THU (Therapeutic use), BIOL (Biological study); PREP (Preparation), USES (Uses)

(testosterone prodrugs for improved drug delivery)

RN 189830-21-5 CAPLUS

CN Androsta-3,5-dien-3,17-diol, bis[4-(trimethylammonio) butanoate], dibromide, (17.beta.)- (9CI) (CA INDEX NAME)

L12 ANSWER 6 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER:
DOCUMENT NUMBER:
INVENTOR(S):

PATENT ASSIGNEE(S):
DOCUMENT TYPE:
LANGUAGE:
DOCUMENT TYPE:
LANGUAGE:
PATENT INFORMATION:

COUNTRY TYPE:
PATENT INFORMATION:

COUNTRY TYPE:
PATENT INFORMATION:

PATENT NO. KIND DATE

PATENT NO. KIND DATE APPLICATION NO. DATE

JP 03059295 A2 19970304 JP 1996-115165 19960510

PRIORITY APPLN. INFO.: JP 1995-1415165 19960512

OTHER SOUNCE(S): MARPAT 126:277656

AB The title compds. [Ir R = Cl-13 alkyl; A = OH or group readily converted to OH; X, Y = wxo, C2-3 alkylenedioxy; X, Y = H, OH, Cl-5 alkoxy, group readily hydrolyzed to OH; however, when X = OH or group readily hydrolyzed to OH; however, when X = OH or group readily hydrolyzed to OH; X must be H, when Y = OH or group readily hydrolyzed to OH; X must be H, when X = Cl-5 alkoxy; Y must be Cl-5 alkoxy; are prepd. Thus, the title compd. II was prepd. in 10 steps from 3.beta., 12.beta.-dihydroxy-5.alpha.-pregnan-20-one and showed an IC50 of 0.0776 .mu.g/mL against XB

It 188488-22-4P la8488-23-59 188488-25-19

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); TRU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of chlorocholestane derivs. as antitumors)

RN 188488-22-4 CAPLUS

CG Glycine, N,M-dimethyl-, (3.beta.,5.alpha.,12.beta.,205,22R)-21-chloro-12,20-dihydroxy-26,27-dinorergostane-3,22-diyl ester, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 6 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN

Absolute stereochemistry.

L12 ANSWER 6 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN

188488-23-5 CAPLUS Glycine, N. N. diethyl-, (3.beta., 5.alpha., 12.beta., 205, 22R)-21-chloro-12, 20-dihydroxy-26, 27-dinorergostane-3, 22-diyl ester, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

188488-25-7 CAPLUS Glycine, N.N-dimethyl-, (3.alpha.,5.alpha.,12.beta.,205,22R)-21-chloro-12,20-dihydroxy-26,27-dinorergostane-3,22-diyl ester, monohydrochloride (9C1) (CA INDEX NAME)

L12 ANSWER 7 OF 41 CAPLUS COPYRIGHT 2003 ACS ON STN ACCESSION NUMBER: 1997:195445 CAPLUS DOCUMENT NUMBER: 126:199709 Anion Recognition by Tricals Anion Recognition by Tripodal Receptors Derived from Cholic Acid
Davis, Anthony P.; Perry, Justin J.; Williams, Robert

Absolute stereochemistry.

RL: PRF (Properties); RCT (Reactant); SFN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

L12 ANSWER 7 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
(anion recognition by tripodal receptors derived from cholic acid)
RN 187730-62-7 CAPLUS
CN Cholan-24-oic acid, 7,12-bis[[[(3,5-dimethylphenyl)amino]carbonyl]oxy]-3[[(4-methylphenyl)sulfonyl]amino]-, methyl ester,
(3.alpha.,5.beta.,7.alpha.,12.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT

187730-73-0P 187730-75-2P 187730-85-4P
187730-87-6P 187730-88-7P
RL: PRP (Properties): SPN (Synthetic preparation): PREP (Preparation)
(anion recognition by tripodal receptors derived from cholic acid)
187730-73-0 CAPLUS
Cholan-24-olc acid, 7,12-bis{[[(3,5-dimethylphenyl)amino]carbonyl]oxy]-3[[(4-methylphenyl)sulfonyl]amino]-, methyl ester,
(3,alpha.5,beta.7,alpha.1/2,alpha.1/2,compd. with N,N,N-tributyl-1butanaminium fluoride (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 187730-62-7 CMF C50 H67 N3 O8 S

Absolute stereochemistry.

L12 ANSWER 7 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

CM

187730-85-4 CAPLUS
Cholan-24-oic acid, 7,12-bis[[[(3,5-dimathylphenyl)amino]carbonyl]oxy]-3[[(4-methylphenyl)sulfonyl]amino]-, methyl ester,
[(3.alpha.,5.beta.,7.alpha.,12.alpha.)-, compd. with N,N,N-tributyl-1butanaminium bromide (1:1) (9CI) (CA INDEX NAME)

CRN 187730-62-7 CMF C50 H67 N3 O8 S

Absolute stereochemistry.

L12 ANSWER 7 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

CM 2

CRN 429-41-4 CMF C16 H36 N . F

• F-

187730-75-2 CAPLUS
Cholan-24-oic acid, 7,12-bis[[[(3,5-dimethylphenyl)amino]carbonyl]oxy]-3[[(4-methylphenyl)aulinoyl)amino]-, methyl ester,
[(3.alpha.,5.beta.,7.alpha.,12.alpha.)-, compd. with N,N,N-tributyl-1butanaminium chloride (1:1) (9CI) (CA INDEX NAME)

CRN 187730-62-7 CMF C50 H67 N3 O8 S

Absolute stereochemistry.

L12 ANSWER 7 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

CM 2

CRN 1643-19-2 CMF C16 H36 N , Br

● Br-

187730-87-6 CAPLUS
Cholan-24-oic acid, 7,12-bis[[[(3,5-dimethylphenyl)amino]carbonyl]oxy]-3[[(4-methylphenyl)sulfonyl]amino]-, methyl ester,
(3.alpha.,5.beta.,7.alpha.,12.alpha.)-, compd. with N,N,N-tributyl-1butanaminium iodide (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 187730-62-7 CMF C50 H67 N3 O8 S

L12 ANSWER 7 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

CM 2

CRN 311-28-4 CMF C16 H36 N . I

• 1-

RN 187730-88-7 CAPLUS
CN Cholan-24-oic acid, 7,12-bis[[[(3,5-dimethylphenyl) amino] carbonyl]oxy]-3[[(4-methylphenyl) sulfonyl] amino]-, methyl ester,
(3.alpha.,5.beta.,7.alpha.,12.alpha.)-, compd. with N,N,N-tributyl-1butanaminium salt with.4-methylbenzenesulfonic acid (1:1:1) (9CI) (CA
INDEX NAME)

CM 1

CRN 187730-62-7 CMF C50 H67 N3 O8 S

Absolute stereochemistry.

L12 ANSWER 7 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN (Continued

CM 2

CRN 7182-86-7 CMF C16 H36 N . C7 H7 O3 S

CM 3

CRN 16722-51-3 CMF C7 H7 O3 S

CM 4

CRN 10549-76-5 CMF C16 H36 N

- P.

n-Bu-N+ Bu-n | | n-Bu

L12 ANSWER 8 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1997:5476 CAPLUS
DOCUMENT NUMBER: 126:104294
TITLE: Steroids 54. Amino acylamidosteroids
AUTHOR(S): Vincze, Iren, Hackler, Laszlo; Szendi, Szuzsa;
Schneider, Gyula
CORPORATE SOURCE: Steroids (1996), 61(12), 697-702

PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: STEDAN; ISSN: 0039-128X

BAB Aminosteroids were prepd. and acylated with protected amino acids by means of the mixed anhydride or the active ester method. The tert-butyloxycarbony1- (80C) protecting group was eliminated by acidolysis, and the benzyloxycarbony1- (2) group by catalytic hydrogenation. 3.beta.-And 6.beta.-Glycylamidosteroids were prepd. by indirect amination of chloroacetamido derivs., formed by the Ritter reaction on the corresponding 3.alpha., 5.alpha., -cyclo and 5.alpha., 6.alpha.-esopxy steroids. Water-sol. double salts were produced from the compds. for pharmacol. investigations.

II 185842-85-7P 185842-86-8P 185842-88-0P

RL: PRP (Properties); SRN (Synthetic preparation); PREF (Preparation)
(prepn. of amino acylamidosteroids)

N 185842-85-7 CAPJUS

CN 1

CN 1

CN 1

CN 1

CN 1

CN 66675-78-3

CNF C23 H38 N2 O2

Absolute stereochemistry. Rotation (+).

CRN 87-69-4 CMF C4 H6 06

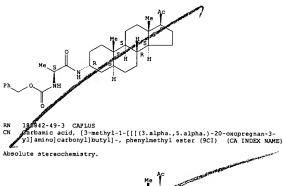
L12 ANSWER 8 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

185842-86-8 CAPLUS
Propanamide, 2-amino-N-[(3.alpha.,5.alpha.)-20-oxopregnan-3-y1]-, (S)-,
(2R,3R)-2,3-dihydroxybutanedioate (2:1) (9CI) (CA INDEX NAME)

CM 1 CRN 107978-52-9 CMF C24 H40 N2 O2

185842-88-0 CAPLUS
Pentanamide, 2-amino-4-methyl-N-[(3.alpha.,5.alpha.)-20-oxopregnan-3-yl]-,
(2R,3R)-2,3-dihydroxybutanedioate (2:1) (9CI) (CA INDEX NAME)

L12 ANSWER 8 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



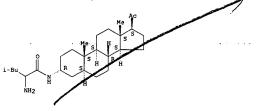
185842-65-3P 185842-67-5P 185842-68-6P 185842-69-7P 185842-71-1P 185842-96-0P 185843-15-6P 185844-59-1P 185844-60-4P ΙT

18584-60-4P
RL: SPN (Synthetic preparation); PREF (Preparation)
(prepn. of amino acylamidosteroids)
185842-65-3 CAPLUS
Glycinamide, glycyl-N-[(3.alpha.,5.alpha.)-20-oxopregnan-3-y1]-,
monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

L12 ANSWER 8 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN CRN 185842-87-9 CMF C27 H46 N2 O2 . .

Absolute stereochemistry.



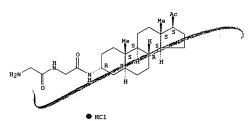
Absolute stereochemistry.

185842-48-2P 185842-49-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Freparation); RACT (Reactant or reagent) (prepn. of amino acylamidosteroids)
185842-48-2 CAPLUS
Carbamic acid, [1-methyl-2-oxo-2-[[(3.alpha.,5.alpha.)-20-oxopregnan-3-yl]amino]ethyl]-, phenylmethyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

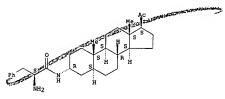
L12 ANSWER 8 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN

(Continued)



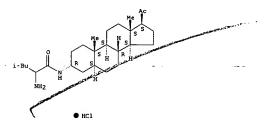
185842-67-5 CAPLUS
Benzenepropanamide, alpha.-amino-N-[(3.alpha.,5.alpha.)-20-oxopregnan-3-yl]-, monohydrochloride, (\$)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



185842-68-6 CAPLUS
Pentanamide, 2-maino-4-methyl-N-[(3.alpha.,5.alpha.)-20-oxopregnan-3-yl]-,
monohydrochloride (9CI) (CA INDEX NAME)

L12 ANSWER 8 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



RN 185842-69-7 CAPLUS
CN Acetamide, 2-amino-N-{(3.beta.)-20-oxopregn-5-en-3-yl}-, monohydrochloride
(9CI) (CA INDEX NAME)

Absolute Stereochemistry. Rotation (+).

RN 185842-71-1 CAPLUS
CN Acetamide, N-[(3.beta.,5.alpha.,6.beta.)-3-(acetyloxy)-5-hydroxy-20oxopregnan-6-yl]-2-amino-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

• HCl

L12 ANSWER 8 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

RN 185843-15-6 CAPLUS
CM Propanamide, 2-amino-N-[(3.alpha.,5.alpha.)-20-oxopregnan-3-yl]-, monohydrochloride, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+)

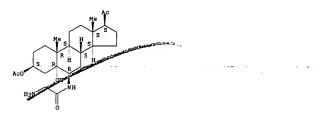
RN 185044-59-1 CAPLUS CN Acetamide, 2-amino-N-[(3.alpha.)-20-oxopregn-5-en-3-y1]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 18584-60-4 CAPLUS CN Acetamide, N-[(3.beta.,5.alpha.,6.beta.)-3-(acetyloxy)-5-hydroxy-20oxopregnan-6-y1]-2-amino- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

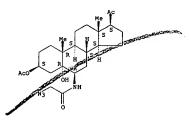
L12 ANSWER 8 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN (Continued



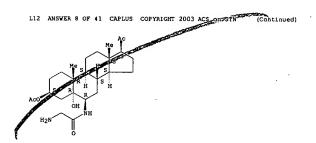
● HCl

RN 185842-96-0 CAPLUS
CN Acetamide, N-[(3.beta.,5.alpha.,6.beta.)-3-(acetyloxy)-5-hydroxy-20cxopregnan-6-yl]-2-azido- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



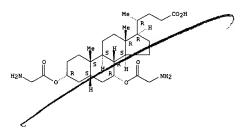
RN 185843-11-2 CAPLUS CN Acetamide, 2-azido-N-[(3.alpha.)-20-oxopregn-5-en-3-yl]- (9CI) (CA INDEX NAME)



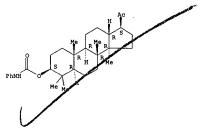
Li2 ANSWER 9 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1996:692070 CAPLUS
COCUMENT NUMBER: 126:60319
TITLE: Sequence-selective nonmacrocyclic two-armed receptors
for peptides
AUTHOR(S): Nestler, H. Peter
CORPORATE SOURCE: Cold Spring Harbor Lab., Cold Springs harbor, NY,
11724, USA
SOURCE: Cold Spring Harbor Lab., Cold Springs harbor, NY,
11724, USA
Molecular Diversity (1996), 2(1/2), 35-40
CODEN: MODIF4; ISSN: 1381-1991
PUBLISHER: ESCOM
DOCUMENT TYPE: Journal
LANGUAGE: All Springs Harbor Lab., Cold Springs harbor, NY,
recognition on several occasions. We decided to make twofold use of this
reception on several occasions. We decided to make twofold use of this
reception on several occasions. We decided to make twofold use of this
reception of the characteristics of the receptors. We prepd. two
small peptides, and secondly to investigated the importance of structural
preorganization for the characteristics of the receptors. We prepd. two
combinatorial tripeptide chains held by different scaffolds: the use of
chenodeoxycholic acid as spacer provided a rigid scaffold for the forceps,
whereas linking the peptide chains by a pentamethylene chain yielded a
very flexible forceps structure. Mols. from the cholic acid library
recognize and discriminate various enkephalins with micromolar affinities.
Mols. from the flexible library show distinct interactions with the
enkephalins as well, but the specificity and affinity are clearly
diminished. Thus, although the interactions of mol. forceps with a
rigid design are clearly superior to flexible mol. forceps
IT 188215-77-40, peptidyl derivs., resin-bound
RL: BPR (Biological process) BSU (Biological study, unclassified); BIOL
(Biological study): PROC (Process)
(Sequence-selective nonmacrocyclic two-armed receptors for peptides)

Absolute stereochemistry.

### Absolute stereochemistry.



L12 ANSWER 10 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN



L12 ANSWER 10 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1996:544204 CAPLUS
DOCUMENT NUMBER: 125:544214
A Short Enantioselective Total Synthesis of
Dammarenediol II S
AUTHOR(S): Corey, E. J., Lin, Shouthong
Department of Chemistry, Harvard University,
Cambridge, MA, 02138, USA
JOURNAL OF MAN (2138, USA
JOURNAL OF MAN (2138, USA)

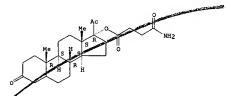
Absolute stereochemistry.

181776-88-5 CAPLUS

10-Norpregnan-20-one, 4,4,8,14-tetramethyl-3-[[(phenylamino)carbonyl]oxy]-, (3.beta.,5.alpha.)- (9CI) (CA INDEX NAME)

L12 ANSWER 11 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1996:405139 CAPLUS
DOCUMENT NUMBER: 125:143123
Synthesis of 17.alpha.-hydroxyprogesterone succinate
bovine serum albumin fluorescein isothiocyanate
2hong, Zhicheng; Sun, Zhenxian; Li, Xiaoqin
SOURCE: Zhong, Zhicheng; Sun, Zhenxian; Li, Xiaoqin
SOURCE: Hamaroy, West China Univ. Med. Sci., Chengdu,
5100411, Peop. Rep. China
DOCUMENT TYPE: CODEN: HYZAEZ; ISSN: 1006-0103
HUSHISHER: Husxi Yike Daxue Yaoxueyuan
JOCUMENT TYPE: Journal
LANGUAGE: Albaha-hydroxyl progesterone-hemisuccinyl-BSA-FITC)
of ER and FR was synthesized from 17.alpha.-hydroxyprogesterone in three
steps: acylation, formation of mix-anhydride, and conjugation to form
complex. The method is simple. The complex of the synthetic was
identified by spectroscope anal.
IT 179683-32-0P
RL: RCT (Reactant); SFN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(synthesis of hydroxyprogesterone succinate bovine serum albumin
fluorescein isothiocyanate)
RN 17968-32-0 CAPLUS
CN Pregn-4-ene-3,20-dione, 17-(4-amino-1,4-dioxobutoxy)- (9CI) (CA INDEX
NAME)

Absolute stereochemistry.



I/9083-32-ODP, conjugate with serum bovine albumin and fluorescein isothiocyanate RE: SPN (Synthetic preparation), PREP (Preparation) (synthesis of hydroxyprogesterone succinate bovine serum albumin fluorescein isothiocyanate) 179683-32-0 CAPLUS Pregn-4-ene-3,20-dione, 17-(4-amino-1,4-dioxobutoxy)- (9CI) (CA INDEX NAME)

L12 ANSWER 11 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

L12 ANSWER 12 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN

179532-28-6 CAPLUS L-Tyrosine, N-[4-[[(11.alpha.)-17,21-dihydroxy-3,20-dioxopregn-4-en-11-yl]oxy]-1,4-dioxobutyl]-3-(iodo-125I)-, methyl ester (9CI) (CA INDEX NAME)

179532-29-7 CAPLUS L-Tyrosine, N-[4-[{(11.beta.)-17,21-dihydroxy-3,20-dioxopregn-4-en-11-yl]oxy}-1,4-dioxobutyl}-, methyl ester (9CI) (CA INDEX NAME)

L12 ANSWER 12 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER:
1996:398816 CAPLUS
117TILE:
125:143118
Radioimmunological and chromatographic properties of tyrosine methyl ester conjugates with stereoisomeric steroid carboxy derivatives.
AUTHOR(S):
Lapcik, Oldrich: Hampl, Richard; Hill, Martin; Starka, Luboslave Kasal, Alexander: Pouzar, Vladimir; Putz, Zdenek
CORPORATE SOURCE:
Local Inst. Endocrinol., Prague, 116 94, Czech Rep.
COllection of Czechoslovak Chemical Communications (1996), 61(5), 799-807
CODEN: CCCCAX; ISSN: 0010-0765
PUBLISHER:
Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic
Journal
LANGUAGE:
Beginsh
AB Pure 32 (syn) and 3E (anti) stereoisomers of testosterone
3-[0-(2-carboxyethyl)] oxine were synthesized, sepd. by HPLC or TLC, and used for prepn. of tyrosine Me ester (TME) conjugates by using mixed anhydride or carbodiimide-N-hydroxysuccinimide methods. While the latter method provided more than 960 of product with retained configuration, the mixed anhydride method yielded a mixt. contg. 26-40% of the opposite stereoisomer. The Streeoisomers were used as model compds., to which the other steroid TMES and the corresponding radioiodinated products could be aligned according to their chromatog, properties. The TME conjugates of 3-(0-carboxymethyl) oximes of seven 4-en-3-oxo steroids were further prepd. by carbodiimide-N-hydroxysuccinimide method. With exception of cortisol, the stereoisomeric (2 and E) radioidinated TME conjugates of the reap. steroid carboxy derivs. with TME and their radioidinated tracers were synthesized from hemisuccinates of cortisol and its 11.alpha.-isomer, via 11.beta.- and 11.alpha.-hydroxy group. The radioidinated TMES did not differ in their binding properties. In the case of isomeric cortisol tracers conjugated through position 11 the antisera raised by using position-homologous conjugates of the resp. steroid carboxy derivs. with bovine serum albumin as immunogens. With the exception of 11-deoxycorticosterone, the stere

179532-30-0P
RL: PRP (Properties); PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation) (prepn., radioimmunol. and chromatog. properties of tyrosine Me ester conjugates with stereoisomeric steroid carboxy derivs.)
179532-27-5 CAPLUS
L-Tyrosine, N-[4-{[(11.alpha.]-17,21-dihydroxy-3,20-dioxopregn-4-en-11-y1]oxy]-1,4-dioxobuty]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 12 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

179532-30-0 CAPLUS L-Tyrosine, N-[4-[[(11.beta.)-17,21-dihydroxy-3,20-dioxopregn-4-en-11-yl]oxy]-1,4-dioxobutyl]-3-(iodo-1251)-, methyl ester (9CI) (CA INDEX NAME)

L12 ANSWER 13 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1996:309980 CAPLUS
DOCUMENT NUMBER: 125:33944
TITLE: The palladium-catalyzed vinylic substitution of vinyl
triflates with .beta.-substituted-.alpha.,.beta.unsaturated carbonyl compounds. An application to the
synthesis of cardenolides
AUTHOR(S): Arcadi, Antonior Cacchi, Sandror Fabrizi, Giancarlo;
Marinelli, Fabio; Pace, Paola
Dip. Chim., Univ. degli Studi, L'Aquila, I-67100,
Italy
SOURCE: Tetrahedron (1996), 52(20), 6983-6996
COODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
CASREACT 125:33944
AB Vinyl triflates react with .beta.-substituted-.alpha.,.beta.-unsatd.
aldehydes, ketones, and esters in the presence of catalytic amts. of
Pd(OAc)2 and an excess of KOAc, omitting phosphine ligands, to give
vinylic substitution products in good to high yield with high
regioselectivity. The added vinyl unit is preferentially linked to the
.beta.-carbon atom. As to the stereochem. vinylic substitution products
contain the carbonyl group on the same side of the preexisting
.beta.-substituent. The use of KOAc has been proved to be superior both
to tertiary amines and to carbonate or bicarbonate bases with or without
the addn. of salts such as LiCl and n-BuAYOL. The application of the
reaction to the synthesis of a cardenolide deriv. In reported. Depending
on the nature of .beta.-substituted-.alpha., beta.-unsatd. carbonyl
compds., tha reaction can produce hydrovinylation (formal conjugated
addn.) products.

IT 17741-19-70
RLI SPN (Synthetic preparation), PREP (Preparation)
(palladium-catalyzed Vinylic substitution of vinyl triflates with

177411-19-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(palladium-catalyzed vinylic substitution of vinyl triflates with .beta.-substituted-.alpha.,beta.-unsatd. carbonyl compds.)
177411-19-7 CAPLUS
Pregna-3,5-dien-20-one, 3-(3-oxo-1-phenyl-1-butenyl)-, [3(2)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

L12 ANSWER 14 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1996:224926 CAPLUS

DOCUMENT NUMBER: 124:311288

Technetium-99m radiolabeled ouabagenin-cysteine
conjugate: Biological evaluation in animal models

Chatterjee, Mitar Ganguly, Shantanur Sarkar, Bharat

R.; Banerjee, Somenath

NUCLEAR HEDICINE DIVISION, INDIAN INSTITUTE CHEMICAL
BIOLOGY, Calcutta, 700 032, India

Nuclear Hedicine and Biology (1996), 23(2), 115-20

CODEN: NMBIEO: ISSN: 0883-2897

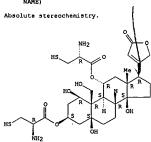
Elsevier

Elsevier Journal English

MAGN. ITE: Journal UAGE: Southal UAGE: English Two ouabagenin-cysteine conjugates were synthesized by condensing 3-.beta. monochloroacetyl and 3-.beta., 11-.alpha. dichloroacetyl ouabagenin with cysteine. The resulting ligands were radiolabeled with technetium-99s (99mTc) to furnish a single homogeneous 99mTc chelate in each case with good stability. The animal expts. with these 99mTc-labeled conjugates established the superiority of guinea pig over rat and rabbit as an animal model, as previously obsd. for other tritiated or radioiodinated cardiac glycosides or alycons. In biodistribution expts. in guinea pig, these 99mTc chelates showed a favorable heart to liver (and other nontarget organ) uptake ratio, comparable to that of recently reported cardioiodinated in animal expts. with ouabagenin derivs. could be attributed to the absence of 3--beta. sugar residues in these mols., which is in agreement with the previous observation reported in connection with radioiodinated digoxin and digoxigenin derivs.

previous observation reported in connection with radioiodinated digoxin and digoxigenin derivs.

176223-45-30P, technetium-99 conjugates
RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); TRU (Therapeutic use); BIOL (Biological study);
PREF (Preparation); PROC (Process); USES (Uses)
(technetium-99m-oubageain-cysteine conjugate biodistribution in animal models for potential heart scintigraphy)
176223-45-3 CAPLUS
Card-20(22)-enolide, 3,11-bis(2-amino-3-mercapto-1-oxopropoxy)-1,5,14,19-tetrahydroxy-, (1.beta.,3.beta.(R),5.beta.,11.alpha.(R))- (9CI) (CA INDEX NAME)



IT 176223-45-3P

L12 ANSWER 13 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

L12 ANSWER 14 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
RL: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT
(Reactant or reagent)
(technetium-99m-oublagenin-cysteine conjugate biodistribution in animal
models for potential heart scintigraphy)
RN 176223-45-3 CAPLUS
CN Card-20(22)-enolide, 3,11-bis(2-amino-3-mercapto-1-oxopropoxy)-1,5,14,19tetrahydroxy-, [1.beta.,3.beta.(R),5.beta.,11.alpha.(R)]- (9CI) (CA INDEX
NAME)

L12 ANSWER 15 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1996:79303 CAPLUS
DOCUMENT NUMBER: 124:165456
TITLE: Sequence-Selective Peptide Binding with a
Encoded Combinatorial Receptor Library
AUTHOR(S): Cheng, Yuani Suenaga, Toshiro Still, W. Clark
Department of Chemistry, Columbia University, New
York, NY, 10027, USA
JOURNET OUDEY, USA
SOURCE: Journal of the American Chemical Society (1996),
118(7), 1813-14
CODEN: JACSAT, ISSN: 0002-7863
AMERICAN CHEMICAL SOCIETY
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Encoded combinatorial split synthesis was used to prepd. a
polymer-supported library consisting of 104 different peptidosteroids (I).
Related compds. are known to bind certain oliopoptides sequence
selectively. The new peptidosteroids have an altered A,B-ring fusion and
are less flexible than those previously described. Screening the library
I for binding of a dye-labeled pentapeptide (5-Leu-enkephalin Me ester
(II)) showed significantly improved binding selectivity. Peptidosteroids
I (V2 = (I)Asn(N-trityl)-(D-)Asn(N-trityl)-Ac, V1 = (D)Phe-X-Ac) that
bound II most strongly showed significantly weaker binding with many 5-Leu
enkephalin derivs. in which single amino acids were changed from the
natural sequence.
IT 173738-17-50, resin bound
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP
(Properties); BIOL (Biological study); PROC (Process)
(peptido-A,B-trans-steroid combinatorial receptor library
sequence-selective enkephalin binding)
RN 173738-17-5 CAPLUS
C Cholan-24-oic acid, 3-[(N-[N-acetyl-0-(1,1-dimethylethyl)-L-sepyl]-Dphenylalanyl] maino]-7-([N2-(N2-acetyl-N-(triphenylmethyl)-L-separaginyl]-N(triphenylmethyl)-L-saparaginyl] amino]-, (3.alpha.,5.alpha.,7.alpha.)(9CI) (CA INDEX NAME)

L12 ANSWER 16 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1996:8289 CAPLUS

DOCUMENT NUMBER: 124:76653

TITLE: Serum binding of steroid tracers and its possible effects on direct steroid immunoassay.

AUTHOR(S): Micallef, Jacob V.; Hayes, Margaret M.; Latif, Abdul; Absan, Rukhsana; Sufi, Saulat B.

CORPORATE SOURCE: World Health Organization Collaborating Centre Research Immunoassay, Hammersmith Hospital, London, W12 OHS, UK

Annale of Clinical Biochemistry (1995), 32(6), 566-74 CODEN: ACBOBU, ISSN: 0004-5632

PUBLISHER: Royal Society of Medicine Press
DOCUMENT TYPE: Journal

LANGUAGE: Royal Society of Medicine Press
DOCUMENT TYPE: Journal

AB The authors studied the serum protein binding of 3H-labeled progesterone, estradiol and testosterone, and five 1251-labeled analogs of these steroids. All tracers investigated appeared to be bound by proteins in every serum sample tested. The addn. of blocking agents caused a substantial redn. in serum protein binding of 3H-labeled steroids, but had relatively little effect on the binding of analog steroid tracers. Use of analog steroid tracers in conventional direct immunoassays for estradiol and progesterone produced anomalous results for some patient samples when compared to extn. RIAs, but assays where tracer binding to serum constituents was prevented by adoption of two-step procedures appeared to avoid anomalous results. The results suggest that serum protein binding of steroid annalog tracers may be a source of interference in some direct steroid immunoassays.

IT 172302-99-7

RL: ARG (Analytical reagent use): BPR (Biological process): BSU (Biological study): PROC (Process): USES (Uses) (Serum binding of steroid tracers and its possible effects on direct steroid immunoassay.

steroid immunoassay)
172302-99-7 CRPLIS
Pregn-4-ene-3,20-dione, 11-[4-[2-[2-(iodo-1251)-1H-imidazol-4-yl]ethyl]amino]-1,4-dioxobutoxy]-, (11.alpha.)- (9CI) (CA INDEX NAME)

L12 ANSWER 15 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN

(Continued) PAGE 1-B

- NH- CPh3

L12 ANSWER 17 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN ACCESSION NUMBER: 1995:652248 CAPLUS DOCUMENT NUMBER: 123:55427

DOCUMENT NUMBER: TITLE: 123:5542/ Preparation of optically active cyclohexane derivatives and other optically active organic

Compounts
Okazaki, Masaki; Uchino, Nobuhiko; Matsuo, Yasushi
Fuji Photo Film Co Ltd, Japan
Jpn. Kokai Tokkyo Koho, 20 pp.
CODEN: JXXXAF INVENTOR(S):

PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE:

Patent

LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

JP 06263704 A2 19940920 JP 1993-52392 19930312

PRIORITY APPLN. INFO: JP 1993-52392 19930312

OTHER SOURCE(S): MARPAT 123:55427

AB The title compds. with chromophores RIRRNCH:CHCH:CKY [R1, R2 = H, alky1, etc.: R1 and R2 may together form a ring; X, Y = electron-attracting group) are prepd. Cyclohexane deriv. I (prepn. given) showed [.alpha.]397 + 25000.degree. and .lambda.max = 364 nm.

11 164366-76-9 164386-78-1

RL: PRF (Properties) (prepn. of optically active cyclohexane derivs. and other optically active org. compds.)

RN 16436-76-9 CARLUS

CN Cholestane-2,3-diol, bis[2-cyano-5-(diethylamino)-2,4-pentadienoate], (2.alpha.,3.beta.,5.alpha.) - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry unknown.

164386-78-1 CAPLUS Cholestane-2,3-diol, 2-[2-cyano-5-(dimethylamino)-2,4-pentadienoate] 3-[5-(diethylamino)-2-(phenylsulfonyl)-2,4-pentadienoate], (2.alpha.,3.beta.,5.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

L12 ANSWER 17 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

164386-82-7 CAPLUS Cholestane-3,6-diol, bis[2-cyano-5-(diethylamino)-2,4-pentadienoate], (S.alpha.,6.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

(CH<sub>2</sub>) 3

L12 ANSWER 18 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN

161579-86-8 CAPLUS Pregn-5-en-20-one, 3-(acetyloxy)-17-[[[(trichloroacetyl)amino]carbonyl]oxy]-, (3.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 18 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1995:271538 CAPLUS
DOCUMENT NUMBER: 122:187861
TITLE: Synthesis of (19E)-3.beta.,17-dihydroxy-20-oxopregn-5-en-19-al 19-(0-carboxymethyl)oxime, new steroidal hapten for 17-hydroxypregnenolone
AUTHOR(S): Pouze, Vladimir, Fajkos, Jan
CORPORATE SOURCE: Inst. Org. Chem. Biochem., Acad. Sci. Czech Republic, Prague, Czech Rep.
SOURCE: Steroids (1994), 59(12), 696-701
CODEN: STEDAM. ISSN: 0039-128X
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANCUAGE: English
AB (19E)-3.beta.,17-dihydroxy-20-oxopregn-5-en-19-al 19-(0-carboxymethyl)oxime was prepd. from 5-bromo-6.beta.,19-epoxy-20-oxo-5.alpha.-pregnan-3.beta.-yl benzoate in 12 steps.

IT 161579-84-6P 161879-85-7P 161879-86-8P
RL: PPR (Properties) SPN (Synthetic preparation), PREP (Preparation) (synthesis of (19E)-3.beta.,17-dihydroxy-20-oxopregn-5-en-19-al 19-(0-carboxymethyl) oxime, new steroidal hapten for 19-hydroxytypregnenolone)
RN 161579-84-6 CAPIUS
CA Acetic acid, [[(3.beta.,19E)-3-(benzoyloxy)-20-oxo-17-[((trichloroacety)) amino] carbonyloxy)-pregn-5-en-19-ylidene] amino] oxy]-, methyl ester (SCI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

161579-85-7 CAPLUS Acetic acid, [[([3.beta.,19E]-3-hydroxy-20-oxo-17-[[([trichloroacety1) amino] carbony1] oxy]pregn-5-en-19-ylidene] amino] oxy]-, methyl ester [9CI] (CA INDEX NAME]

Absolute stereochemistry.
Double bond geometry as shown.

L12 ANSWER 19 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN ACCESSION NUMBER: 1995:237598 CAPLUS DOCUMENT NUMBER: 122:23370

DOCUMENT NUMBER: TITLE:

122:23370
Interaction of an estramustine photoaffinity analog with cytoskeletal proteins in prostate carcinoma cells Speicher, Lisa A.; Laing, Naomi; Barone, Linda R.; Robbins, Joan D.; Seamon, Kenneth B.; Tew, Kenenth D. Dep. Pharmacology, Fox Chase Cancer Center, Philadelphia, PA, 1911, USA Molecular Pharmacology (1994), 46(5), 866-72 CODEN: MOPNA3; ISSN: 0026-895X Williams & Vilkins AUTHOR (S):

CORPORATE SOURCE:

SOURCE:

PUBLI SHER:

PUBLISHER:

Williams & Wilkins
DOCUMENT TYPE:

Journal
ANGUAGE:

English
AB To identify specific drug targets of the antimitotic drug estramustine, a photoaffinity analog, 17-0-[12-[3-(4-azido-3-[1251]iodophenyl]propionamido | sthyllcarbamyl]estradiol-3-N-bis(2-chlorosthyl)carbamate [1] was synthesized and reacted in competition assays with cytoskeltal protein prepns. By attaching the photoaffinity ligand to the 17.beta.-position of the steroid D-ring, the cytotoxic properties of the drug were maintained. In cytoskeltal protein prepns. From human prostate carcinoma cells (DU 145) or a clonally selected, estramustine-resistant cell line (E4), the major microtubule-assocd. protein (MAP) present was MAP4. In both cytoskeltal fractions and reconstituted microtubules, I bound to both MAP4 and tubulin. From competition assays, the apparent binding const. for MAP4 from DU 145 cells was 15. mw.M. Similar calcus. for tubulin gave values of 13. mm.M (E4 cells). The identification of these cytoskeletal proteins as specific drug targets provides a direct explanation for the antimicrotubule and antimitotic effects of estramustine.

IT 159859-38-49

Ri: RCT (Reactant); SPN (Synthetic preparation); PREF (Preparation); PACT

13989-38-49
RE: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT (Reactant or reagent) (in preparation): RACT (in preparation): 15989-38-4 CAPLUS Estra-1, 3,5 (10) -triene-3,17-diol (17.beta.)-, 17-[(2-aminoethyl)carbamate] 3-[bis(2-chloroethyl)carbamate] (SCI) (CA INDEX NAME)

Absolute stereochemistry.

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SFN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

L12 ANSWER 19 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
(interaction of estramustine photoaffinity analog with cytoskeletal proteins in prostate carcinoma cells)
RN 159899-37-3 CAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol (17.beta.)-, 17-[[2-[[3-[4-azido-3-(iodo-1251)phenyl]-1-oxopropyl]amino]ethyl]carbamate] 3-[bis(2-chloroethyl)carbamate] (9CI) (CA INDEX NAME)

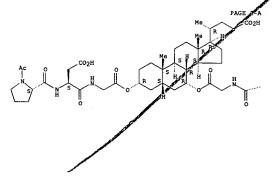
Absolute stereochemistry.

L12 ANSWER 20 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN

PAGE 1-B

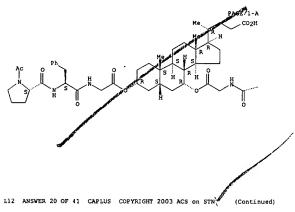
161419-35-8 CAPLUS
Cholan-24-oic acid, 3,7-dihydroxy-, (3.fwdarw.1)-ester with
N-(N-(1-acety]-L-pcolyl)-L-.alpha.-aspartyl]glycine, 7-ester with
N-[1-(N-acetyl-L-val)-L-prolyl]glycine, (3.alpha.,5.beta.,7.alpha.)
(9CI) (CA INDEX NAME)

## Absolute stereochemistry.



L12 ANSWER 20 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1995:45102 CAPLUS
DOCUMENT NUMBER: 122:188108
TITLE: Peptidosteroidal Receptors for Opioid Peptides.
Sequence-Selective Binding Using a Synthetic Receptor
Library
AUTHOR(S): Boyce, Rustum; Li, Ge; Nestler, H. Peter; Suenaga,
Toshiro; Still, W. Clark
CORPORATE SOURCE: Department of Chemistry, Columbia University, New
York, NY, 10027, USA
SOURCE: Journal of the American Chemical Society (1994),
116(17), 7955-6
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
English
AB Peptidosteroids I (PS = polystyrene; V1 = Ac-AA1-AA2-Gly and V2 =
Ac-AA3-AAW where AA = amino acid residues) were prepd. in 104 different
forms by encoded combinational chem. Using a series of enkephalin-like
opioid psptides as substrates, different substrates preferentially bind
different members of the above peptidosteroid receptor library.
IT 161419-34-7DP, aminomethyl polystyrene resin-bound
161419-36-9DP, aminomethyl polystyrene resin-bound
161419-36-9DP, aminomethyl polystyrene resin-bound
161419-39-7DP, aminomethyl polystyrene resin-bound
161419-39-7DP, aminomethyl polystyrene resin-bound
161419-39-POP, aminomethyl polystyrene
161419-39-POP, aminomethyl polystyrene
1

#### Absolute stereochemistry.



PAGE 1-B

161419-36-9 CAPLUS Cholan-24-oic acid, 3,7-dihydroxy-, 3-ester with N-{N-(N-acetyl-L-alanyl}-L-phenylalanyl]glycine, 7-ester with N-{1-(N-acetyl-L-valyl)-L-ptoxyl]glycine, (3.alpha.,5.beta.,7.alpha.)- (9CI) (CA INDEX NAME)

L12 ANSWER 20 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN

(Continued)

161419-37-0 CAPLUS Cholan-24-oic acid, 3,7-dihydroxy-, 3-ester with N-[N-(N2-acetyl-L-lysyl)-L-phenylalanyl]glycine, 7-ester with N-[N-(1-acetyl-L-prolyl)-L-phenylalanyl]glycine, (3.alpha.,5.beta.,7.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 20 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN

(Continued)

PAGE 1-B

Absolute stereochemistry.

PAGE 1-B

L12 ANSWER 20 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN

(Continued)

PAGE 1-B

\_ СО2Н

161419-38-1 CAPLUS
Cholan-24-oic acid, 3,7-dihydroxy-, (3.fwdarw.1)-ester with
N-[N-(N-acetylglycyl)-L-.alpha.-aspartyl]glycine, 7-ester with
N-[N-(N-acetylglycyl)-L-valyl]glycine, (3.alpha.,5.beta.,7.alpha.)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 21 OF 41
ACCESSION NUMBER:
DOCUMENT NUMBER:
1171LE:
INVENTOR(S):

PATENT ASSIGNEE(S):
SOURCE:

COULDENT TYPE:
DOCUMENT TYPE:
LANGUAGE:
FAMILY ACC. NUM. COUNT:
PATENT FORMATION:
FATENT FORMATION:
COPPLIED
COPP

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PAT	ENT N	w.		KIN	ID	DATE			AP	PLIC	ATIC	N N	ο.	DAT	E			
					-													
	42326			A)		19940	331		DE	199	2-42	326	56	199	20929			
DE	42326	556		C2		19950	1112											
EP	59048	39		A2		19940	1406		EP	199	3-11	524	7	199	30922			
EP	59048	39		A3		19940	629											
EP	59048	9		В1		19963	211											
			BE,						GB, G	GR,	ΙE,	IT,	LI,	LU	, MC,	NL,	PT,	SE
AT	14618	34		E		1996:	1215		AT	199	3-11	524	7	199	30922			
	20955			Т3		19970			ES	199	3-11	524	7	199	30922			
JP	06211	1893		A2		19940	2080		JP	199	3-24	336	0	199	30929			
US	55211	l 67		A		19960	528		US	199	3-12	812	8	199	30929			
PRIORITY	APPI	LN. I	NFO.	. :					DE 199	92-4	232€	556		199	20929			
OTHER SO																		
AB Tit	le co	mpds	3. [I	[ ; dc	tte	d lir	nes :	indi	cate :	ging	le c	r d	oubl	e b	onds:	х =	0.	5;
R =	subs	titi	ited	alky	1.	alker	111	R1 -	- (sul	ostí	tute	d)	arvl	. m	ono-	or		

N - Substituted alky, alkenyl Ni - (Substituted) alkyl, alkenyl], were prepd. biheterocyclyl; R2 -4H, Me, (Substituted) alkyl, alkenyl], were prepd. Thus, 17.alpha.-(3-furyl)-5.beta.-androstan-3.beta.,17.beta.-diol was condensed with 1-(2-chloroethyl)pyrrolidine using NaH in THF to give 3.beta.-[2-(1-pyrrolidinyl)ethoxy]-17.alpha.-(3-furyl)-5.beta.-androstan-17.beta.-ol. I at 20 mg/kg orally in spontaneously hypertensive rats reduced systolic blood pressure from 171 mm Hg (controls) to 148-153 mm

reduced systolic blood pressure from 1/1 mm ny (control),
Hg.
Hg.
159078-99-6P 159079-08-0P 159079-17-1P
159079-26-2P 159079-35-3P 159079-35-3P 159079-17-1P
159079-80-3P 159079-62-6P 159079-91-1P
159080-07-6P 159000-16-7P 159000-25-8P
159080-34-9P
RL: BAC (Biological activity or effector, except adverse), BSU (Biological study, unclassified), SPN (Synthetic preparation), TRU (Therapeutic use),
BIOL (Biological study), PREP (Preparation), USES (Uses)
(prepn. of, as cardiovascular agent)
159078-99-6 CAPLUS
Ethanamine, 2,2'-[[(3.beta.,5.beta.,17.alpha.)-21,23-epoxy-24-norchola-20,22-diene-3,17-diyl]bis(oxy)]bis- (9CI) (CA INDEX NAME)

L12 ANSWER 21 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

159079-08-0 CAPLUS Ethanamine, 2,2'-[[(3.beta.,5.alpha.,17.alpha.)-21,23-epoxy-24-norchola-20,22-diene-3,17-diyl}bis(oxy)}bis- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

159079-17-1 CAPLUS Ethanamine, 2,2'-[[(3.beta.,17.alpha.)-21,23-epoxy-24-norchola-4,20,22-triene-3,17-diyl]bis(oxy)]bis- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 21 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

159079-44-4 CAPLUS Ethanamine, 2,2'-[[(3;beta.,5.alpha.,17.alpha.)-21,23-epithio-24-norchola-20,22-diene-3,17-diyl]bis(oxy)]bis- (9CI) (CA INDEX NAME)

159079-53-5 CAPLUS Ethanamine, 2,2'-[[(3.beta.,17.alpha.)-21,23-epithio-24-norchola-4,20,22-triene-3,17-diyl]bis(oxy)]bis- (9CI) (CA INDEX NAME)

L12 ANSWER 21 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

159079-26-2 CAPLUS Ethanamine, 2,2'-[[(3.beta.,17.alpha.)-21,23-epoxy-24-norchola-5,20,22-triene-3,17-diyl]bis(oxy)]bis- (9CI) (CA INDEX NAME)

159079-35-3 CAPLUS Ethanamine, 2,2'-[[M3.beta.,5.beta.,17.alpha.)-21,23-epithio-24-norchola-20,22-diene-3,17-diyl]bis(oxy)]bis-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 21 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
RN 159079-62-6 CAPLUS
CN Ethanamine, 2,2'-[[(3.beta.,17.alpha.)-21,23-epithio-24-norchola-5,20,22triene-3,17-diyl]bis(oxy)]bis- (9CI) (CA INDEX NAME)

159079-71-7 CAPLUS
Ethanamine, 2,2'-[[(3.beta.,5.beta.,17.beta.)-17-(4-chlorophenyl)androstane-3,17-diyl]bis(oxy)]bis- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

159079-80-8 CAPLUS Ethanamine, 2,2'-[[(3.beta.,5.alpha.,17.beta.)-17-(4-chlorophenyl)androstane-3,17-diyl]bis(oxy)]bis- (9CI) (CA INDEX NAME)

L12 ANSWER 21 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

RN 159079-89-7 CAPLUS
CN Ethanamine, 2,2'-[[(3.beta.,17.beta.)-17-(4-chlorophenyl)androst-4-ene3,17-diyl]bis(oxy)]bis-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 159079-98-8 CAPLUS
CN Ethanamine, 2,2'-[([3.beta.,17.beta.)-17-(4-chlorophenyl)androst-5-ene
3,17-diyl]bis(oxyl)bis- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

RN 159080-25-8 CAPLUS
CN Ethanamine, 2,2'7[(3.beta.,17.beta.)-17-(4-methoxyphenyl)androst-4-ene3,17-diyl]bis(oxy)]bis- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 159080-34-9 CAPLUS
CN /Ethanamine, 2,2'-[[(3.beta.,17.beta.)-17-(4-methoxyphenyl)androst-5-ene'3,17-diyl]bis(oxy)]bis- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 21 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

RN 159080-07-6 CAPLUS
CN Ethanamine, 2,2'-[[(3.beta.,5.beta.,17.beta.)-17-(4-methowyphenyl)androstane-3,17-diyl]bis(oxy)]bis- (9CI) (CA INDEX NAME)

RN 159080-16-7 CAPLUS
CN Ethanamien, 2,2'-[[(3.beta.,5.alpha.,17.beta.)-17-{4methoxyphenyllandrostane-3,17-diyl]bis(oxy)]bis- (9CI) (CA INDEX NAME)
Absolute stereochemistry.

L12 ANSWER 21 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

KIND DATE PATENT NO. APPLICATION NO. DATE

PATENT NO. KIND DATE APPLICATION NO. DATE

GB 2273096 Al 19940608 GB 1992-25235 19921202
GB 2273096 B2 19960605

FRIGHTY APPLM. INFO.: GB 1992-25235 19921202
OTHER SOURCE(S): MARPAT 121:280958
AB COMPGE(S): MARPAT 121:280958
AD 121:280958
A

Absolute stereochemistry.

L12 ANSWER 22 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN

158870-04-3 CAPLUS
Pregn-5-ene-16-acetic acid, 3-(acetyloxy)-.alpha.-(2-mpthyl-1-oxopropyl)20-oxo-.alpha.-(phenylseleno)-, ethyl ester, [3.beta./16.alpha.(R)]- (9CI)
(CA INDEX NAME)

158870-05-4 CAPLUS
Pregn-5-ene-16-acetic acid, 3-(acetyloxy)-.alpha.-(2-methyl-1-oxopropyl)20-oxo-.alpha.-(phenylseleno)-, ethyl ester, [3.beta.,16.alpha.(5)]- (9CI)
(CA INDEX NAME)

158870-05-5F 158870-07-6F
RL: SPM (Synthetic preparation); PREP (Preparation)
(prepn. of piperidoazaandrostanone derivs. as testosterone
5.alpha.-reductase inhibitors)
15870-06-5 CAPLUS
Pregn-5-ene-16-acetic acid, 3-(acetyloxy)-.alpha.-(2-methyl-1-oxopropyl)-20-oxo-, ethyl ester, [3.beta.,16.beta.(R)]- (9CI) (CA INDEX NAME)

L12 ANSWER 22 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN

158869-91-1 CAPLUS Pregn-5-ene-16-acetic acid, 3-(acetyloxy)-.alpha.-(2-methyl-1-oxopropyl)-20-oxo-, ethyl ester, (3.beta.,16.alpha.(5))- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

158869-92-2 CAPLUS Pregn-5-en-20-one, 3-hydroxy-16-(3-methyl-2-oxobutyl)-, (3.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

158869-93-3 CAPLUS Pregn-4-ene-3,20-dione, 16-(3-methyl-2-oxobutyl)-, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry

ANSWER 22 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN (Continued) Absolute stereochemistry.

158870-07-6 CAPLUS
Pregn-5-ene-16-acetic acid, 3-(acetyloxy)-.alpha.-(2-methyl-1-oxopropyl)20-oxo-, ethyl ester, [3.beta.,16.beta.(S)]- (9CI) (CA INDEX NAME)

L12 ANSWER 23 OF 41 CAPLUS COPYRIGHT 2003 ACS ON STN ACCESSION NUMBER: 1994:622331 CAPLUS DOCUMENT NUMBER: 121:222331

TITLE:

121:222331
Photoaffinity labeling with progesterone-11.alpha.-hemisuccinate-(2-[1251]iodohistamine) identifies four protein bands in mouse brain membranes Bukusoglu, Cuneytr Krieger, Neil R. Department of Anesthesia, Brigham and Women's Hospital, Boston, MA, USA
Journal of Neurochemistry (1994), 63(4), 1434-8
CODEN: JONRA9; ISSN: 0022-3042
Journal AUTHOR(S):

CORPORATE SOURCE:

SOURCE:

DOCUMENT TYPE:

CODEN: JONRA9, ISSN: 0022-3042

DOCUMENT TYPE: Journal
LANGUAGE: Replish
AB The radiolabeled progesterone (PG) analog progesterone-11.alpha.hemisuccinate-(2-[125]iodohistamine) was used to label PG binding
proteins in brain membranes from mours cerebellum. Photosffinity labeling
and SDS-PAGE identified specific PG binding protein bands 1-4 of 64-29
kDa. Bands 1 and 4 were well resolved on the gel and easily quantified.
Preincubation with PG inhibited photolabeling in a dose-dependent manner.
The labeling was specific with respect to steroid structure. For band 1,
the extent of inhibition of labeling by PG and J.alpha., Salpha.pregnanolone (3.alpha.) was pronounced. Other steroids such as
testosterone (Tes), estradiol (ESt), and corticosterone (Cor) were less
effective, whereas pregnenolone sulfate (PS) and cholesterol (Coh) were
ineffective. With respect to band 4, ESt was the most effective PG,
3.alpha., and Tes were intermediate; and PS, Cho, and Cor were
ineffective. The results describe specific membrane proteins that bind PG
(band 1) and ESt (band 4).

IT 18922-23-4
RE: ARG (Analytical reagent use); BAC (Biological activity or effector,
except adverse); BSU (Biological study, unclassified); ANST (Analytical
study); BIOL (Biological study); USES (Uses)
(photoaffinity labeling of steroid binding proteins of cerebellum
membranes by)
RN 18522-23-4 CAPLUS
CN Pregn-4-ene-3,20-dione, 11-[4-[[2-(2-iodo-1H-imidazol-4-yl)ethyl]amino]1,4-dioxobutoxyl-, (11.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 24 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN ACCESSION NUMBER: 1994:509398 CAPLUS

1994:509398 121:109398 DOCUMENT NUMBER:

TITLE:

121:109398
Preparation of 17-aryl- and 17-heterocyclyl5.beta.,14.beta.-androstanes as cardiovascular agents
Almirante, Nicoletta, Bernardi, Luigi, Cerri, Alberto,
Melloni, Piero; Padoani, Gloria, Quadri, Luisa
Sigma-Tau Industrie Farmaceutiche Riunite S.p.A.,
Italy
Ger. Offen., 13 pp.
CODEN: GWXXEX
Patent
German
1 INVENTOR(S): PATENT ASSIGNEE(S):

SOURCE:

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PAT	TENT NO.	1	KIND	DATE	APPLICATION NO.	DATE
DE	4232638		A1	19940331	DE 1992-4232638	19920929
DE	4232638		C2	19941117		
EP	590272		A2	19940406	EP 1993-112500	19930804
EP	590272		A3	19940706		
EP	590272		B1	19970102		
	R: AT,	BE, CI	i, DE,	DK, ES,	FR, GB, GR, IE, IT, I	LI, LU, MC, NL, PT, SE
AT	147077		E	19970115	AT 1993-112500	19930804
ES	2095531		т3	19970216	ES 1993-112500	19930804
CA	2106917		AA	19940330	CA 1993-2106917	7 19930924
ZA	9307085		Α	19940811	ZA 1993-7085	19930924
JP	06192286		A2	19940712	JP 1993-243359	19930929
US	5567694		A	19961022	US 1993-128114	19930929
ORITY	Y APPLN.	INFO.:			DE 1992-4232638	19920929

US 5567694 A 1996102 US 1993-12011 19930929
PRIORITY APPLM. INFO.: DE 1992-422638 19920929
OTHER SOURCE(s): MARPAT 121:109398 19920929

AB Title compds. [1] R - aryl, heterocyclyl; 1 of Y = OH, OR3, SR3 and the other - H; Y2 = O, NNRC(HNINE); R1-R3 = H, alk(en)yl, acyl, etc.; dashed line = optional bond) were prepd. Thus, 17.beta.-phenyl-5.beta.-androst-15-ene-3.beta.; 14.beta., 17.alpha.-triol was converted in 5 steps to 3.beta.-(3-aminopropoxy)-17.beta.-phenyl-5.beta.-androstana-14.beta., 17.alpha.-diol which had pIC50 of 4.6 against Na+, Kx-ATPase.

IT 156721-98-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study); PREF (Preparation); THU (Therapeutic use); BIOL (Biological study); PREF (Preparation); USES (Uses) (prepn. of, as cardiovascular agent)

RN 156721-98-1 CAPUUS

Androstan-14-ol, 3,17-bis(3-aminopropoxy)-17-phenyl-, (3.beta.,5.beta.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 25 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1994:316018 CAPLUS
DOCUMENT NUMBER: 1994:316018 CAPLUS

AUTHOR(S): Binding of homologous and heterologous isoluminol- and enzyme-labeled progesterone conjugates to monoclonal antibodies

AUTHOR(S): De Boever, Jozef G.; Kohen, Fortune; Bosmans, Eugene Department of Obstetrics and Gynacology, University Hospital, Ghent, B. 9900, Belg.
Analytica Chimica Acta (1994), 290(1-2), 239-45
CODEN: ACACAM; ISSN: 0003-2670

DOCUMENT TYPE: Journal
LANGUAGE: English
AB The binding of three different progesterone-rayme (RRP) conjugates to monoclonal antibodies against progesterone-rayme (RRP) and progesterone 11. The insuccinate bridges at carbon atom 3, 7 or 11. The enzyme labels were covalently bound to progesterone via henisuccinate bridge at carbon atom 3, 7 or 11. The enzyme labels were covalently attached to the steroid using a carboxymethyl-aminocaproic acid bridge at carbon atom 3 or a hemisuccinate bridge at carbon atom 11. The influence of several factors on the binding between antibodies and conjugates and on the slopes of the calibration curves was studied. Considerable differences in the binding of the label and in the shape of the curves was governed by the presence in the reaction mixt. of the antibodies in liq. or solid-phase conditions.

RN 155515-11-0 CAPLUS
CN Pregn-4-ene-3, 20-dione, 7-(4-{{2-[ethyl{1},2,3,4-tetrahydro-1,4-dioxo-6-phthalazinyl) aminolethyl]sminol-1,4-dioxobutoxyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

155515-12-1 CAPLUS
Pregn-4-en-20-one, 3-[4-[{2-(ethyl{1,2,3,4-tetrahydro-1,4-dioxo-6-phthalazinyl)amino]ethyl]amino]-1,4-dioxobutoxy]- (9CI) (CA INDEX NAME)

L12 ANSWER 25 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN

(Continued)

PAGE 1-A

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L12 ANSWER 26 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1994:253366 CAPLUS
DOCUMENT NUMBER: 120:253366
TITLE: Compositions and methods for enhanced drug delivery
Hale, Ron L., Lu, Amy; Solas, Dennis; Selick, Harold
E., Oldenburg, Kevin R., Zaffaroni, Alejandro C.
Affyman Technologies N.V., Neth.
PCT int. Appl., 155 pp.
CODENET TYPE: Patent
LANGUAGE: PIXXO2
PATENT INFORMATION:

PATENT INFORMATION:

PATENT INFORMATION:

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

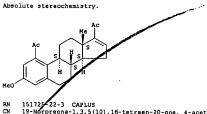
WO 93325197 A1 19931223 WO 1993-US5631 19930611
W. AT, AU, BB, BG, BR, CA, CH, CZ, DE, DN, ES, FI, GB, HU, JP, KP,
KR, LK, LU, MG, MN, WW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SK,
UA, US
RY: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE,
BF, BJ, CF, CG, CI, CM, GA, M, ML, MR, NE, SN, TD, TG
AU 9345345 A1 19940104 AU 1993-45345 19930611
R: CH, DE, FR, GB, IT, LI, NL
US 5607691 A 19970304 US 1995-449188 19950524
PRIORITY APPLN. INFO:

US 1993-9463 19930127
WO 1993-US5631 19930611
US 1993-164293 19931029

AB The present invention relates to methods of delivering pharmaceutical agents across membranes, including the skin layer or mucosal membranes of a patient. A pharmaceutical agent is covalently bonded to a chem.
modifier, via a physiol. cleavable bond, such that the membrane transport and delivery of the agent is enhanced. Propesterone 3-{2-0-(10-0-0)-acetyl-a-cranitine acid chloride (prepn., given). In vitro serum half-lives of some pharmaceutical agent-chem. modifier complexes are given.

IT 184279-48-8
RI: BIOL (Biological study)
(as drug-chem. modifier conjugate through physiol. cleavable bond, for enhanced drug transport across membranes)

RN 154279-48-8 CAPLUS
CN Pregnan-20-one, 3-{3-(acetyloxy)-1-oxo-4-(trimethylammonio)butoxy}-,
[3.beta.(R),5.alpha.]- (SCI) (CA INDEX NAME)
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N 19-Norpregna-1,3,5(10),16-tetraen-20-one, 4-acetyl-3-methoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 27 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

725-21-2P AL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of) 151725-21-2 CAPLUS 19-Norpregna-1,3,5(10),16-tetraen-20-one, 2-acetyl-3-methoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 29 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1993:444589 CAPLUS
DOCUMENT NUMBER: 119:44589
P-Maleimidophenyl isocyanate: a novel heterobifunctional linker for hydroxyl to thiol

AUTHOR (S):

heterobifunctional linker for mystomy to that coupling Annunziato, Michael E.; Patel, Usha S.; Ranade, Madhuri; Palumbo, Paul S.
PB Diagn. Syst., Inc., Westwood, MA, 02090, USA Bioconjugate Chemistry (1993), 4 (3), 212-18 CODEN: BCCHES; ISSN: 1043-1802 CORPORATE SOURCE:

DOCUMENT TYPE:

CODEN: BCCHES; ISSN: 1043-1802

MENT TYPE: Journal
UNAGE: English
P-Maleinidophenyl isocyanate (PMPI, 1) is a heterobifunctional
crosslinking agent useful for thiol to hydroxyl coupling. Several
maleinide-activated compds. were preped, and characterized and then shown
to be reactive with thiol-contg. proteins. Examples include activation of
vitamin B12, digoxigenin, digitoxigenin, estradiol, progesterone, and some
serine-contg. peptides.
146528-51-2P
RL: PREP (Preparation)

146528-51-2P
RE: PREP (Preparation)
(prepn. of)
148528-51-2 CAPLUS
Pregn-4-ene-3, 20-dione, 11-[[[[4-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-y1)phenyl]amino]carbonyl]oxy]-, (11.beta\*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 28 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1993:650230 CAPLUS
DOCUMENT NUMBER: 1993:650230 CAPLUS
CONVERSION OF VARIABLE STORES
AUTHOR(S): CONVERSION OF VARIABLE STORES
AUTHOR(S): Arcadi, Antonio Cacchi, Sandro Marinelli, Fabio Dip. Chim. Ing. Chim. Mater., Univ. L'Aquila, L'Aquila, 1-67100, Italy
SOURCE: CODEN: TETRAB: ISSN: 0040-4020
DOCUMENT TYPE: Journal English
LANGUAGE: English
CASREACT 119:250230
AB Vinyl triflates have been converted into .gamma.'-hydroxy-.alpha.,.beta-enones through their palladium-catalyzed coupling with 1-butyn-4-ols followed by the reaction of the obtained 1-hydroxy-3-yn-5-enes in an acidic CH2C12/3N HCl two-phase system in the presence of the n-BuNGC1/Pdc12 combination. Both the coupling step and the conversion of the carbon-carbon triple bond into the ketonic group have been performed at room temp. Thus, the Pd-catalyzed coupling of vinyl triflate I (Tf triflate) with 1-butyn-4-ol gave 93 1-hydroxy-3-yn-5-enes II, which was converted to 791 .gamma.-hydroxy-.alpha.,.beta.-enone III in an acidic CH2C12/3N HCl two-phase system in the presence of n-BuNGC1/Pdc12. The conversion of vinyl triflates into .gamma-hydroxy-.alpha.,.beta.-enones acan be carried out through a one-flask process, without the isolation of 1-hydroxy-3-yn-5-enes.

IT SIT2-03-IP
RL: SPN (Synthetic preparation); PREF (Preparation) (prepn. of, via palladium-catalyzed coupling reaction of vinyl triflate

1011/2-03-IP (Synthetic preparation): PREP (Preparation) (prepn. of, via palladium-catalyzed coupling reaction of vinyl triflate with butynol)

CAPLUS

Pregna-3,5-dien-20-one, 3-(4-hydroxy-1-oxobutyl)- (9CI) (CA INDEX NAME)

Absolute.stereochemistry.

L12 ANSWER 30 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN ACCESSION NUMBER: 1993:248540 CAPLUS DOCUMENT NUMBER: 118:248540 GABAA receptor with steroid bin Als: 248540
GABAA receptor with steroid binding sites and agonists and drug screening methods
Gee, Kelvin Wellman; Lan, Nancy Tsail Yun
Cocensys, Inc., USA
PCT Int. Appl., 62 pp.
CODEN: PIXXD2
Patent

INVENTOR(S): PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE: Patent

English

LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO. KIND DATE

WO 9305786 A1 19930401 WO 1992-U57613 19920909

W: AU, CA, JP, KR
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, SE
AU 9226572 A1 19930427 AU 1992-26572 19920909

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, SE
JP 0653102 A1 19940629 EF 1992-920306 19920909

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, SE
JP 05510999 T2 19941208 JP 1992-506095 19920909

PRIORITY APPLN. INFO.: US 1991-759512 19910913

WO 1992-US7613 19920909

WO 1992-US7613 19920909 APPLICATION NO. DATE

NRITY APPLN. INFO:

US 1991-759512
19910913
A. gamma.-aminobutyric acid (GABA)A receptor-chloride ionophore complex (GRC) is disclosed which has a GABAA-associd. neurostercid receptor (GRR). The GRR may, depending on the binding agent used, reside on the .alpha.-beta. subunit combination of the GRC. Agonists of the GNR on the GRC are claimed and are useful for treating anxiety, seizures, mood disorders, premenstrual syndrome, post natal depression, and insomnia. A method for screening for drugs that bind to GNRs with different subtype specificity comprises expressing CDNA encoding GRC subtypes in cells to form an expressed GNR subtype and screening for agonists of that subtype. A competitive or an allosteric modulatory assay may be used. The therapeutic index (LDS):EDSO) for 3.alpha.-hydroxy-5.alpha.-pregnan-20-one (3.alpha.-OH-DHP) is >122 when based on the EDSO against (+) bicuculline-induced seizures, thus indicating very low toxicity and good anticonvulsant activity. Modification of the 3.alpha.-position of 3.alpha.-OH-DHP with an acetate, propionate, or butyrate group increased the time of protection provided against seizures in mice. 147850-40-6, 3.alpha.-Acetyl-5.alpha.-pregnan-20-one
147850-41-7, 3.alpha.-Butyryl-5.alpha.-pregnan-20-one
147850-42-8, 3.alpha.-Butyryl-5.alpha.-pregnan-20-one
147850-40-6 CARIUS
Pregnan-20-one, 3.acetyl-, (3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

L12 ANSWER 30 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

CAPLUS (1-ожоргору1)-, (3.alpha.,5.alpha.)- (9СІ) (СА INDEX

7850-42-8 CAPLUS RN CN regnan-20-one, 3-(1-oxobutyl)-, (3.alpha.,5.alpha.)- (9CI) (CA INDEX AME)

te stereochemistry Ab

ANSWER 31 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN

L12 ANSWER 31 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1992:524780 CAPLUS
DOCUMENT NUMBER: 117:124780

AUTHOR(S): Pregnane derivatives as pregnancy interceptive agents: efficacy determination on growing trophoblasts (in vitro) and in pregnant hamsters (in vivo) shukla, Rajiv, Mehrotra, P. X., Deivedi, A., Kamboj, V. P.
CORPORATE SOURCE: Div. Endocrinol., Cent. Drug Res. Inst., Lucknow, 226 001, India
SOURCE: Contraception (1992), 45(6), 605-15 COOMS. CCPTAY, ISSN: 0010-7824
DOCUMENT TYPE: Journal English

COEN: CCPTAY; ISSN: 0010-7824

DOCUMENT TYPE: Journal
LANGUAGE: English

AB An in vitro test system was standardized to study potentiality of five hormonally inert pregnane derivs. on growing trophoblasts isolated from ectoplacental cone (EPC) of day 8 hamster embryo. Cells were incubated with different concens of resp. compds. in surface droplets. The response was detd. by analyzing the sequence of changes in cell morphol. like attachment, growth, proliferation, differentiation and/or degeneration within 24 or 48 h following seedling. The in vivo efficacy of these compds. was detd. in hamster during peri- and immediate post-implantation periods (days 3-8 post coitum). Two compds. 88/583 and 88/585 were found to inhibit not only growth and proliferation of the cells but caused total degeneration within 24 h. The same compds. induced partial to complete resorption of the fetuses in treated animals. Whereas, the other three compds. 88/506, 88/594 and 89/43 that showed lack of comparable potentiality in vitro were found to be equally ineffective in vivo. The results indicate a pos. correlation between in vitro and in vivo activity.

IT 134329-78-5 143324-344

RL: BIOL (Biological study)
(pregnancy interception by)
134329-78-5 CAPLUS

(pregnancy interception by)
134329-78-5 CAPLUS
19-Norpregna-1,3,5(10)-trien-20-one, 1-[3-(diethylamino)-2-hydroxypropoxy]4-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

143328-45-4 CAPLUS 19-Norpregna-1,3,5(10)-trien-20-one, 1-[3-(diethylamino)propoxy]-4-methyl-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 32 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER:
1991:651330 CAPLUS
TITLE:
115:251330 The effect of estramustine derivatives on microtubule assembly in vitro depends on the charge of the substituent
Priden, Bor Rutberg, Mikael, Deinum, Johannar Wallin,
Margareta
CORPORATE SOURCE:
Dep. Zoophysiol., Univ. Goeteborg, Goeteborg, S-400
31, Swed.
SOURCE:
Biochemical Pharmacology (1991), 42(5), 997-1006
CODEN: BCPCA6; ISSN: 0006-2952
DOCUMENT TYPE:
LANGUAGE:
LOCAL BESTEAMUSTINE INDIBITION OF STREET OF STRE

RL: ANST (Analytical study)
(microtubule assembly response to, ionic charge of substituents in

relation to) 127527-04-2 CAPLUS

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L12 ANSWER 32 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN

L12 ANSWER 33 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN (Continued) L12 ANSWER 33 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER:
DOCUMENT NUMBER:
1991:492696 CAPLUS
115:92696
Synthesis and evaluation of antiinflammatory
activities of a series of corticosteroid
17.alpha.-esters containing a functional group
Ueno, Hiroakir Maruyama, Akira; Miyake, Motoyoshi;
Nakao, Etsuko; Nakao, Kenichiro; Umezu, Kohei; Nitta,
Issei Nakao, austro. Hann, Han CORPORATE SOURCE: SOURCE: DOCUMENT TYPE: LANGUAGE: OTHER SOURCE(S): 133871-61-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREF (Preparation)
(prepn. and antiinflammatory activity of)
133871-61-1 CAPLUS Pregna-1,4-diene-3,20-dione, 21-chloro-17-(3-cyano-1-oxopropoxy)-9-fluoro-11-hydroxy-16-methyl-, (11.beta.,16.beta.)- (9CI) (CA INDEX NAME) Absolute stereochemistry.

L12 ANSWER 34 OF 41
ACCESSION NUMBER:
DOCUMENT NUMBER:
1991:409109 CAPLUS
115:9109
Regioselective reactions of 1,2-dehydroprogesterone:
syntheses of pregnane derivatives as possible
contragestational agents
Decorporate Source:
SOURCE:
DOCUMENT TYPE:
DOCUMENT TYPE:

CAPLUS COPYRIGHT 2003 ACS on STN
1991:409109 CAPLUS
115:9109
Regioselective reactions of 1,2-dehydroprogesterone:
syntheses of pregnane derivatives as possible
contragestational agents
Decorporate Source:
Document Type:

DOCUMENT TYPE:

LANGUAGE:

Steroids (1991), 56(4), 189-94

CODEN: STEDAM; ISSN: 0039-128X

JOHENT TYPE: Journal

JOHENT TYPE: Journal

English

Various pregnane derive. were synthesized from 1, 2-dehydroprogesterone

(I). Ring A of I was aromatized without affecting C-20, and the resulting acetoxy compd. II (R = Ac, Rl = H) after hydrolysis yielded

1-hydroxy-4-methyl-19-norpregna-1,3,5(10)-trien-20-one II (R = Rl = H)

(III). Reactions of III with alkyl halides and 1-chlorc-2,3-epoxypropane gave ethers, e.g., II [R = (CH2)2NEt2, Rl = H] and epoxide IV. Opening of the oxirane ring of IV with secondary amines furnished amino alcs.

Friedel-Craft's acylation of III with maleic anhydride and chloroacetyl chloride gaver II [R = H Rl = COCH:CHCO2H, COCHEC1 (V)] resp. Reaction of I with triethyl orthoformate in the presence of boron trifluoride etherate involved the participation of C-21, and the carbonyl at C-3 remained unaffected. The product was identified as 21-[2-hydroxyvinyl]-21-norpregna-1,4-diene-3,20-dione. Reductive amination of I with sodium cyanoborohydride in the presence of ammonium acetate did not attack ring A and smoothly furnished 20-aminopregna-1,4-dien-3-one, which, on reaction with succinic anhydride, gave the succinamide. Other derivs. of I, III, 184328-19-65

RCT (Reactant), SPN (Synthetic preparation); PREP (Preparation); RACT

134329-79-69
REL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and esterification of, with methanol) 134329-79-6 CAPLUS 2-Butenoic acid, 4-(1-hydroxy-4-methyl-20-oxo-19-norpregna-1,3,5(10)-trien-2-yl)-4-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry unkn

134329-80-9P 134329-80-99 / RL: RCT (Reactant), SPN (Synthetic preparation), PREP (Preparation), RACT (Reactant or reagent) (prepn. and intramol. cyclization of, cyclopentaphenanthrofuran from) 134329-80-90 CAPLUS 19-Norpregna-1,3,5(10)-trien-20-one, 2-(chloroacetyl)-1-hydroxy-4-methyl-

L12 ANSWER 34 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN (9CI) (CA INDEX NAME) (Continued)

Absolute stereochemistry.

134329-76-3P 134329-78-5P 134329-85-4P
134329-86-5P 134329-87-6P
RL: SPN (Synthetic preparation), PREP (Preparation)
(prepn. of)
134329-76-3 CAPLUS
19-Norpregna-1,3,5(10)-trien-20-one, 1-[2-(diethylamino)ethoxy]-4-methyl(9CI) (CA INDEX NAME)

Absolute stereochemistry.

139<sup>3</sup>29-78-5 CAPLUS 19-Norpregna-1,35(10)-trien-20-one, 1-[3-(diethylamino)-2-hydroxypгороху)-4-methyl- (9C1) (CA INDEX NAME)

L12 ANSWER 34 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
RN 134329-07-6 CAPLUS
CN 19-Norpregna-1,3,5(10)-trien-2-butanoic acid, 1-hydroxy-.beta.-methoxy-4methyl-.gamma.,20-dioxo-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 34 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN

134329-85-4 CAPLUS
13-Norpregna-1,3,5(10)-trien-20-one, 1-[3-[bis(1-methylethyl)amino]-2-hydroxypropoxy]-4-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

134329-86-5 CAPLUS
2-Butenoic acid, 4-(1-hydroxy-4-methyl-20-oxo-19-norpregna-1,3,5(10)-trien-2-yl)-4-oxo-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry unknown.

L12 ANSWER 35 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1990:514769 CAPLUS

DOCUMENT NUMBER: 1990:514769 CAPLUS

TITLE: Synthesis and structure-activity relationships of N.N'-di-o-tolylguanidine analogs, high-affinity ligands for the haloperidol-sensitive .sigma. receptor Scherz, Michael W.; Fialeix, Michelle Fischer, James B.; Reddy, N. Lawars Server, Alfred C.; Sonders, Mark S.; Tester, Barbara C.; Weber, Eckard: Wong, Scott T.; Keana, John F. W.

CORPORATE SOURCE: Dep. Chum., Univ. Oregon, Eugene, OR, 97403, USA Journal of Medicinal Chemistry (1990), 33(9), 2421-9 CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal of Medicinal Chemistry (1990), 33(9), 2421-9 CODEN: JMCMAR; ISSN: 0022-2623

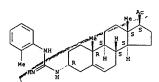
DOCUMENT TYPE: Journal of Medicinal Chemistry (1990), 33(9), 2421-9 CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal of Medicinal Chemistry (1990), 33(9), 2421-9 CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal of Medicinal Chemistry (1990), 33(9), 2421-9 CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: JOURNAL OF THE STRUCK OF THE

Absolute stereochemistry.



128414-00-6 CAPLUS
Guanidine, N-(2-methylphenyl)-N'-[(3.alpha.}-20-oxopregn-5-en-3-yl]-,
monohydrochloride (9CI) (CA INDEX NAME)

L12 ANSWER 35 OF 41 CAPLUS - COPYRIGHT 2003 ACS on STN • HCl

L12 ANSWER 36 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

127527-14-4P 127527-15-5P 127527-16-6P

127527-17-P 127527-13-8P 127527-19-9P

127527-20-2P 127527-23-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as antineoplastic)

RN 127527-05-3 CAPLUS

CN Glycine, N-methyl-, (17.beta.)-3-[[[bis(2-chloroethyl)amino]carbonyl]oxy]e

stra-1,3,5(10)-trien-17-yl ester, monoethanesulfonate (9CI) (CA INDEX NAME) CM 1.

CRN 127527-04-2 CMF C26 H36 C12 N2 O4

Absolute stereochemistry.

127527-07-5 CAPLUS Glycine, (17.beta.)-3-{{{bis(2-chloroethy1) amino] carbony1}oxy]estra-1,3,5(10)-trien-17-yl ester, monomethanesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 127527-06-4 CMF C25 H34 C12 N2 O4

Absolute stereochemistry.

L12 ANSWER 36 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER:
1990:406678 CAPLUS
113:6678
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113: DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

DATES NO	WIND	2000	100.1015.00	
PAIENI NO.		DAIL	APPLICATION NO.	DATE
			EP 1989-111062	19890619
EP 351561		19931027	a. 1505 11100E	.,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,
			GR, IT, LI, LU, NL	. SE
US 5036062	A		US 1989-365436	
CA 1317587	A1	19930511	CA 1989-603014	19890616
AT 96446	E	19931115	AT 1989-111062 ES 1989-111062	19890619
ES 2059626	Т3	19941116	ES 1989-111062	19890619
AU 8936682	A1	19900104	AU 1989-36682	19890621
AU 607621 ZA 8904716	B2	19910307		
ZA 8904716	Α	19900328	ZA 1989-4716	19890621
DK 8903189	A		DK 1989-3189	
NO 8902672 NO 172939	A	19891229	NO 1989-2672	19890627
NO 172939	В	19930621		
NO 172939	С	19930929		
FI 8903130	A		FI 1989-3130	19890627
FI 92707	В	19940915		
FI 92707	Ç	19941227		
JP 02053795	A2		JP 1989-162850	19890627
JP 2563587		19961211		
HU 52521		19900728	HU 1989-3235	19890627
HU 203766		19910930		
CN 1045792		19901003	CN 1989-104490	19890627
CN 1031060	В	19960221		
DD 284026	A5	19901031	DD 1989~330011	19890627
RU 2036929			RU 1989-4614513	
LT 3548			LT 1993-603	
LV 10235		19950420		19930608
PRIORITY APPLN. INFO	.:		SE 1988-2402	
			EP 1989-111062	19890619

L12 ANSWER 36 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

HO-- CH3

127527-10-0 CAPLUS Glycine, N-methyl-, (17.beta.)-3-[[[bis(2-chloroethyl)amino]carbonyl]oxy]e stra-1,3,5(10)-trien-17-yl ester, monohydrochloride (9CI) (CA INDEX NAME)

L12 ANSWER 36 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
RN 127527-11-1 CAPLUS
CN Glycine, N-methyl-, (17.beta.)-3-[[bis(2-chloroethyl)amino]carbonyl)oxyle
stra-1,3,5(10)-trien-17-yl ester, monomethanesulfonate (9CI) (CA INDEX
NAME)

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CRN 127527-04-2 CMF C26 H36 C12 N2 O4

Absolute stereochemistry.

CM

CRN 75-75-2 CMF C H4 O3 S

127527-12-2 CAPLUS Glycine, N,N-dimethyl-, (17.beta.)-3-[[[bis(2-chloroethyl)amino]carbonyl]oxy]estra-1,3,5(10)-trien-17-yl ester, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 36 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN . (Continued)

● HC1

127527-15-5 CAPLUS Estra-1, 3,5(10)-triene-3,17-diol (17.beta.)-, 3-[bis(2-chloroethyl)carbamate] 17-[4-(dimethylamino)butanoate], monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

HC1

127527-16-6 CAPLUS Glycine, N-ethyl-, (17.beta.)-3-{[[bis(2-chloroethyl)amino]carbonyl]oxy]estra-1,3,5(10)-trien-17-yl ester, monohydrochloride (9CI) (CA INDEX NAME)

L12 ANSWER 36 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

● HC1

127527-13-3 CAPLUS Glycine, (17.beta.)-3-[[[bis(2-chloroethyl)amino]carbonyl]oxy]estra-1,3,5(10)-trien-17-yl ester, monohydrochloride (9C1) (CA INDEX NAME)

Absolute stereochemistry.

127527-14-4 CAPLUS L-Alanine, (17.beta.)-3-[[[bis(2-chloroethyl)amino]carbonyl]oxy]estra-1,3,5(10)-trien-17-yl ester, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 36 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN

• HC1

127527-17-7 CAPLUS
Glycine, N-propyl-, (17.beta.)-3-{{{bis{2-chloroethyl}amino|carbonyl}oxyle
stra-1,3,5(10)-trien-17-yl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HC1

127527-18-8 CAPLUS Glycine, N-(1-methylethyl)-, (17.beta.)-3-[{[bis(2-chlorosthyl) amino]carbonyl]oxy]estra-1,3,5(10)-trien-17-yl ester, nonohydrochloride (9CI) (CA INDEX NAME)

L12 ANSWER 36 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

● HC1

127527-19-9 CAPLUS Glycine, N-[1,1-dimethylethyl)-, {17.beta.}-3-[[bis(2-chloroethyl)amino]carbonyl]oxy]estra-1,3,5(10)-trien-17-yl ester, monhydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

• HC1

127527-20-2 CAPLUS Glycine, N., d-diethyl-, (17.beta.) -3-[[[bis(2-chloroethyl)amino]carbonyl)ox y|estra-1,3,5(10)-trien-17-yl ester, monohydrochloride (9CI) (CA INDEX NAME)

L12 ANSWER 37 OF 41 CAPLUS COPYRIGHT 2003 ACS ON STN

ACCESSION NUMBER: 1990:51377 CAPLUS

DOCUMENT NUMBER: 112:51377 CAPLUS

AUTHOR(S): Potential tumor or organ imaging agents. 31.
Radioiodinated sterol benzoates and carbamates

AUTHOR(S): Van Dort, M.; Santay, L.; Schwendner, S. W.; Counsell, R. E.

CORPORATE SOURCE: Med. Sch., Univ. Michigan, Ann Arbor, MI, 48109-0626, USA

SOURCE: Nuclear Medicine and Biology (1989), 16(6), 603-7

CODEN: NMBIEO; ISSN: 0883-2897

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 112:51377

AB A series of radioiodinated benzoate and carbamate esters of cholesterol and pregnenolone wherein the acyl moiety served as the carrier for radioiodine was synthesized and evaluated as potential imaging agents for the adrenal cortex. 2,6-Dimethyl-3-lodobenzoyl and N-(4-iodophenyl) carbamoyl groups were chosen as the acyl functionality in an attempt to provide esters resistant to in vivo hydrolysis. Tissue disposition studies in rats revealed that their biodistribution as detd. by the attached sterol carrier; the cholesterol esters demonstrated significant uptake at 24 h in the adrenal whereas the corresponding pregnenolone derivs. showed only slight affinity for steroid-secreting tissues at this time.

IT 124784-19-6P

time.

12474-19-6F
RL: BPR (Biological process); BSU (Biological study, unclassified); SPN
(Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC
(Process)
(prepn. and metab. of, scintigraphy of adrenal cortex in relation to)

(Process) (prepn. and metab. of, scintigraphy of adrenal cortex in relation to) 124704-19-6 CAPLUS (Prepn.-Sen-20-one, 3-[[[[4-(iodo-1251)phenyl]amino[carbonyl]oxy]-, (3.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. 1251

124824-72-0P
RL: 301 (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and radiolodination of) 124824-12-0 CAPLUS Pregn-5-en-20-one, 3-[[[(4-iodophenyl)amino]carbonyl]oxy]-, (3.beta.)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

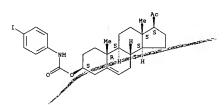
L12 ANSWER 36 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN

• HCl

127527-23-5 CAPLUS
.beta.-Alanine, (17.beta.)-3-[[[bis(2-chloroethyl)amino]carbonyl]oxy]estra1,3,5(10)-trien-17-yl ester, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 37 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



L12 ANSWER 38 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1990:7791 CAPLUS
TITLE: 112:7791
INVENTOR(S): 12:7791 Pregnane derivatives useful as intermediates for vitamin D3 derivatives, and their preparation Tsuji, Jiror Takahashi, Takashi; Tsuji, Masaor Nakagawa, Naoshir Takigawa, Tetsuo Kuraray Co., Ltd., Japan
SOURCE: EUR. Pat. Appl., 245 pp.
CODEN: EPXXDW
Patent
LANGUAGE: Patent
FAMILY ACC. NUM. COUNT: 2 FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

1	PAT	ENT	N	٥.		KIN	ďΒ	DATE			API	LICAT	ION	NO.	DATE	
							-									
1	EΡ	321	572	2		A1	l	1989	0628		EP	1988-	902	929	19880	329
1	ΞP	321	572	2		B1	l	1993	0609							
		R:	1	۱T,	BE,	CH,	DE,	FR,	GB,	IT, L	I, 1	IL, SE	:			
1	AΤ	903	57			E		1993	0615		AT	1988-	902	929	19880	329
	JS	535	909	55		A		1994	1025		US	1991-	799	186	19911	127
RIOR	TY	' AP	PL	١.	INFO.	:				JP	198	37-778	49		19870	330
										JP	198	37-778	50		19870	330
										JP	198	37-778	51		19870	330
										JP	198	37-805	89		19870	331
										JP	198	8-805	88		19870	331
										JP	198	37-805	88		19870	331
										EP	198	8-902	929		19880	329
										WO	198	8-JP3	13		19880	329
										US	198	8-283	927		19881	130
										US	190	00-545	120		19900	615

Wo 1988-JP313 19880329
US 1988-ZB3927 19881130
US 1988-ZB3927 19881130
US 1988-ZB3927 19881130
US 1988-ZB3927 19881130
US 1989-ZB3927 19881130
US 2 = H of 21 = H of 21

123946-55-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of, as intermediate for vitamin D3 derivs.)
123946-55-4 CAPLUS
Pregn-5-ene-20-carboxaldehyde, 3-(methoxymethoxy)-1,7-bis[[(phenylamino)carbonyl]oxy]-, cyclic 20-{1,3-propanediyl acetal},

L12 ANSWER 39 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1960:86588 CAPLUS
DOCUMENT NUMBER: 54:1648Dh-i,16481a-c
TITLE: 16-(Substituted-methyl)pregnenolones and derivatives
MAZUE, Robert H.; Cella, John A.
FATENT ASSIGNEE(S): 6. D. Searle & Co.
PATENT ASSIGNEE (S): Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

PATENT NO. KIND DATE APPLICATION NO. DATE

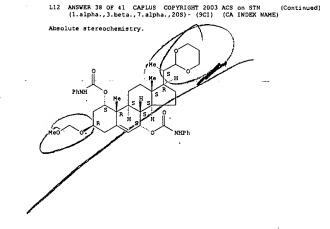
US 2932655 19600412 US

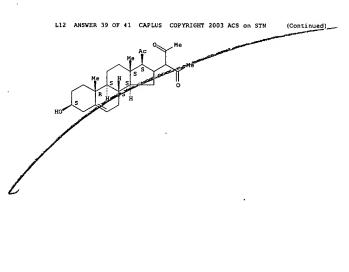
TO K 13 in tert-BuOH 335 at room temp. is added malononitrile 22 then
3.beta.-acetoxypregna-5.16-dien-20-one 60 washed into the reaction with
tert-BuOH 335, the mixt. stirred, refluxed under N overnight, neutralized
with NOAc 20 parts, the solvent removed in vacuo, the residue extd. With
CHC13, the ext. washed with H2O, dried, the CHC13 distd., and the residue
chromatographed on silica gel with C6H6-EtOAc as developing solvents to
give a mixt. of .alpha- and .beta.-isomers of 3.beta.-acetoxy-16(dicyanomethyl)pregn-5-en-20-one, m. 160-90.degree. (anhyd. alc.). To
anhyd. EtOH 1000 is added 3.beta.-acetoxypregna-5,16-dien-20-one 100, Na
14, and malononitrile 40 parts, the mixt. stirred at room temp. until a
clear soln. results, the soln. allowed to stand undisturbed 24 hrs., dild.
with a large vol. of H2O, extd. with CHC13, the CHC13 evapd., and the
residue chromatographed on silica gel with C6H6-EtOAc as developing
solvent to give 16-dicyanomethyl-3.beta.-hydroxypregn-5-en-20-one,
17, freshly distd. cyclohexanone 170, and 204 (iso-PrO)3Al 100 in dry
toluene is added to dry toluene 1500, the mixt. refluxed 2 hrs., cooled,
added to 504 aq. K Na tartrate 1500 parts, the mixt. steam-distd., the
residue extd. with CHC13, the ext. evapd. to dryness, and the residue
chromatographed on silica gel to give 16-dicyanomethylpregn-4-ene-3, 20dione when developed with 104 EtOAc in CGH6, m. 206-10 degree.
(CGH6-cyclohexane). Prepd. similarly are: 3.beta.-acetoxy-16diacetylmethyl) pregn-5-en-20-one, no. 182-6.degree., 16-diacetylmethyl
3.beta.-hydroxypregn-5-en-20-one, 182-6.degree., 16-diacetylmethyl
1-3.beta.-hydroxypregn-5-en-20-one, 182-6.degree., 16-diacetylmethyl
1-3.beta.-hydroxypregn-5-en-20-one, 16-(islacetylmethyl) pregn-4-ene-3, 20dione; the .alpha- and .beta.-isomers of 3.beta.-acetoxy-16(bis(ethoxycarbonyl) methyl) pregn-5-en-20-one, one 150-7.degree.

16-(isleha-cyclohexane). methyl pregn-6-en-20-one, one 150-7.degree.

16-(islpha-(ethoxyc

124320-18-9, 2,4-Pentanedione, 3-(3.0018-3.7,018-3), 16-y1)(prepn. of)
124320-18-9 CAPLUS
2,4-Pentanedione, 3-(3.beta.-hydroxy-20-oxopregn-5-en-16-y1)- (6CI) (CA INDEX NAME)





L12 ANSWER 40 OF 41 CAPLUS COPYRIGHT 2003 ACS ON STN
ACCESSION NUMBER: 1957:81859 CAPLUS
DOCUMENT NUMBER: 5:1:81859
CORIGINAL REFERENCE NO.: 5:1:81859
TITLE: 2,21-Dialkoxalylprogesterones
PATENT ASSIGNEE(S): Upjohn Co.
DOCUMENT TYPE: Patent
LANGUAGE: Patent
Unavailable
PAMILY ACC. NUM. COUNT:
PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO: DATE

GB 761528 19561114 GB

Br (7.4 g.) in 74 ml. MeOH added dropwise during 30 min. to 8 g. II and 5.9 g. anhyd. KOAc in 140 ml. MeOH at 0.degree., and the resulting mixt., contg. the 2,21,21-873 deriv., treated with 50 mg. PhOH and 67 ml. 1.5N

NAOMe in MeOH, heated 5 min. on a steam bath, and added to H20 gave a ppt. of 6.77 g. impure Me 2-bromo-3,11-dioxo-4,17(20) -pregnadien-21-oate (III), purified by chromatography on Florisil and recrystn. from MeOH, primms, m. 155-60.degree. or 160-2.degree., depending upon the rate of heating.

Similarly is produced the 2-Cl analog of III. Also prepd. were alkyl 2-bromo-3-oxo-4,17(20)-pregnadien-21-oates and the 11.alpha.- and 11.beta.-H0 derivs. thereof.

124202-80-8. Androst-4-ene-17.beta.-crotonic acid, 2-(carboxyhydroxymethylene)-.alpha.-hydroxy-.gamma.,3-dioxo-, diethyl ester, di-Na deriv.

(prepn. of)

124202-80-8 CAPLUS

Androst-4-ene-17.beta.-butyric acid, 2-carboxycarbonyl-.alpha.,.gamma.,3-trioxo-, diethyl ester, disodium deriv. (6CI) (CA INDEX NAME)

L12 ANSWER 41 OF 41 CAPLUS COPYRIGHT 2003 ACS on STN

L12 ANSWER 41 OF 41 CAPLUS COPYRIGHT 2003 ACS ON STN
ACCESSION NUMBER: 1957:81858 CAPLUS
DOCUMENT NUMBER: 51:81859
CAPLUS
S1:81859
S1:8185

PATENT NO. KIND DATE APPLICATION NO. DATE

GB 761527 (CO2Et)2 (19 ml.), 21.2 ml. 2.2N NaOMe in MeOH, and 6.9 g.
11-oxoprogesterone (1) in 100 ml. anhyd. Me3COH initially at 50.degree. kept 3 hrs. at room temp., and the pptd. Na dienolate filtered off, dissolved in H2O, and acidified gave 10.2 g. 2, 21-diethoxalyl-11-coxoprogesterone (11), yellow amorphous provder. Also prepd. were 2,21-diethoxalylprogesterone and the 11.alpha.-and 11.beta.-H0 derivs. thereof.
124202-67-1, Androst-4-ene-17.beta.-crotonic acid, 2-(carboxyhydroxymethylene)-alpha-hydroxy-gamma.,3,11-trioxo-, diethyl ester, di-Na deriv. 124202-80-8, Androst-4-ene-17.beta.-crotonic acid, 2-(carboxyhydroxymethylene)-alpha,-hydroxy-gamma.,3-dioxo-, diethyl ester, di-Na deriv.

(prepn. of i-Na deriv.
124202-67-1 CAPLUS
Androst-4-ene-17.beta.-butyric acid, 2-carboxycarbonyl-alpha.-gamma.,3,11-tetraoxo-, diethyl ester, di-Na deriv.

(6CI) (CA INDEX NAME)

●2 Na+

124202-80-8 CAPLUS
Androst-4-ene-17.beta.-butyric acid, 2-carboxycarbonyl-.alpha.,.gamma.,3-trioxo-, diethyl ester, disodium deriv. (6CI) (CA INDEX NAME)

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# (FILE 'HOME' ENTERED AT 09:22:03 ON 07 OCT 2003)

	FILE	'REGISTRY' ENTERED AT 09:22:26 ON 07 OCT 2003
L1		STRUCTURE UPLOADED
L2		2 S L1
L3		566 S L1 FULL
L4		566 S L1 RAN=(123946-55-4,)
L5		566 S L3 OR L4
L6		STRUCTURE UPLOADED
L7		163 S L6 FULL SUB=L5
L8		403 S L5 NOT L7
L9		455 S L5 AND 1/NC
L10		132 S L7 AND 1/NC
	FILE	'CAPLUS' ENTERED AT 10:01:59 ON 07 OCT 2003
L11		125 S L5
L12		41 S L11 NOT PY>=1998

L39 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2003 ACS ACCESSION NUMBER: 2000;567849 CAPLUS DOCUMENT NUMBER: 133:322041 TITLE: Preparation and Charac

Preparation and Characterization of Cholic Acid-Derived Antimicrobial Agents with Controlled Stabilities

Acid-Derived Antimicrobial Agents with Controlled Stabilities

AUTHOR(S):

Guan, Qunying, Li, Chunhong, Schmidt, Erica J., Boswell, J. Scott, Walsh, Joshua P., Allman, Glenn W., Savage, Paul B.

CORPORATE SOURCE:

Departments of Chemistry and Biochemistry and Microbiology, Brigham Young University, Provo, UT, -84602, USA

Organic Letters (2000), 2(18), 2837-2840

CODEN: ORLEFT, ISSN: 1523-7060

PUBLISHER:

American Chemical Society

DOCUMENT TYPE:

LONGUAGE:

American Chemical Society

DOCUMENT TYPE:

JOURNAIN AND A CONTROL OF THE ACT OF THE AC

Absolute stereochemistry.

302784-51-69
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (Preparation); RACT (Reactant or reagent) (Preparation); Raction of cholic acid-derived antimicrobial agents with controlled stabilities) 302784-51-6 CAPLUS (Cholan-24-oic acid, 3,7,12-tris[[[[(1,1-dimethylethoxy)carbonyl]amino]acet

L39 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2003 ACS ACCESSION NUMBER: 1996:692070 CAPLUS DOCUMENT NUMBER: 126:60319

126:60319
Sequence-selective nonmacrocyclic two-armed recep
for peptides
Nestler, H. Peter
Cold Spring Harbor Lab., Cold Springs harbor, NY,
11724, USA
Molecular Diversity (1996), 2(1/2), 35-40
CODEN: MODIF4, ISSN: 1381-1991
SECOM TITLE: selective nonmacrocyclic two-armed receptors

AUTHOR(S): CORPORATE SOURCE:

SOURCE:

PUBLISHER:

DOCUMENT TYPE: LANGUAGE:

CODEN: MODIF4; ISSN: 1361-1991

LISHER: ESCOM

MENT TYPE: Journal

JUAGE: English

Tweezer-like receptor mols. have proven their potential for mol.

Tweezer-like receptor mols. have proven their potential for mol.

Trecognition on several occasions. We decided to make twofold use of this

recognition on several occasions. We decided to make twofold use of this

receptor design: firstly to learn whether simple mol. forceps consisting

of two peptide chains linked by a spacer are able to selectively bind to

small peptides, and secondly to investigated the importance of structural

preorganization for the characteristics of the receptors. We prepd. two

combinatorial tripeptide chains held by different scaffolds: the use of

chenodeoxycholic acid as spacer provided a rigid scaffold for the forceps,

whereas linking the peptide chains by a pentamethylene chain yielded a

very flexible forceps structure. Mols. from the cholic acid library

recognize and discriminate various enkephalins with micromolar affinities.

Mols. from the flexible library show distinct interactions with the

enkephalins as well, but the specificity and affinity are clearly

diminished. Thus, although the interactions of mol. forceps with peptides

are not crucially dependent on structural preorganization, receptors with

a rigid design are clearly superior to flexible mol. forceps.

185215-77-40, peptidyl derivs., resin-bound

Alt. SPR (Biological process): SSU (Biological study, unclassified); BIOL

(Biological study), PROC (Frocess)

(sequence-selective nonmacrocyclic two-armed receptors for peptides)

185215-77-40. CAPLUS

Cholan-24-oic acid, J.,7-bis[(aminoacetyl)oxy]-,

(3.alpha.)-5.beta.,7.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 3 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued) yl]oxy]-, (3.alpha.,5.beta.,7.alpha.,12.alpha.)- (9CI) (CA INDEX NAME) Absolute stereochemistry

REFERENCE COUNT:

14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L39 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2003 ACS ACCESSION NUMBER: 1995:994155 CAPLUS DOCUMENT NUMBER: 124:56726 TITLE: Preparation 5 Preparation of synthetic receptors and libraries Preparation or synthetic receptors and libraries thereof.

Still, W. Clark; Li, Ge: Wennemers, Helma
Trustees of Columbia University in the City of New
York, USA
PCT Int. Appl., 141 pp.
CODEN: PIXXD2 INVENTOR(S): PATENT ASSIGNEE(S): DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION: Patent English 1

9519567 A1 19950720 W0 1995-US572 19950113
W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, C2, DE, DK, EE, ES, FI,
GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG,
MN, MW, MX, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT,
UA, US
RW: KE, MW, SD, S2, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU,
MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN,
TD, TG
2180844 AA 19950720 PATENT NO. KIND DATE WO 9519567 CA 2180844 AU 9521565 AU 686785 AA A1 B2 19950720 CA 1995-2180844 19950113 AU 1995-21565 19950113 19950801 19980212 AU 686785 BZ 175001.1.

2A 9500260 A 19950928 ZA 1995-260
EP 739486 AI 19961030 EP 1995-914675 19950113

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE
JP 09511486 T2 19971118 JP 1995-519163 19950113

IIS 5804563 A 19980908 US 1996-628972 19960408

US 1994-181628 19940113

19950113 PRIORITY APPLN. INFO .:

US 1996-628972 19960408
US 1994-181628 19940113
WO 1995-US572 19960408
WO 1995-US572 19960408
US 1994-181628 19940113
ER SOURCE(S): MARPAT 124:56726
Synthetic receptors comprising a polyfunctional org. template covalently linked to two or more oligomers which may independently be the same or different and may independently be straight chain, cyclic or branched, were prepd. Preferably, the template is covalently linked to a solid support which is linked to an identifier. Libraries of synthetic receptors and methods for assaying synthetic receptor libraries to det. suitable synthetic receptor(s) which (a) bind an acceptor mol.; (b) exhibit biol. activity; (c) which catalyze a reaction or inhibit a catalyzed reaction; and (d) sep. compds. in chromatog, are described. Combinatorial libraries (II P = polymer support; Al-A = Ala, val, Leu, Phe, Pro, Ser, Thr, Lys, Glu, Asp) were prepd. using FMOC chem.; several members of the library were found to bind Leu-enkephalin and Met-enkephalin very selectively. 171762-33-7P OTHER SOURCE(S):

RL: SPN (Synthetic preparation); PREP (Preparation) (preps. of synthetic receptors and libraries thereof) 171762-33-7 CAPLUS

Glycine, N-(N-acetyl-L-phenylalanyl)-, (3.alpha.,5.beta.,7.alpha.)-7-([(acetylamino)acetyl)oxy]-23-carboxy-24-norcholan-3-yl ester (9CI)

L39 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued)

L39 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2003 ACS

PAGE 1-B

161419-35-8 CAPLUS
Cholan-24-oic acid, 3,7-dihydroxy-, (3.fwdarw.1)-ester with
N-[N-(1-acetyl-1-vpclyl)-1-, alpha.-aspartyl]glycine, 7-ester with
N-[1-(N-acetyl-1-valyl)-1-prolyl]glycine, (3.alpha.,5.beta.,7.alpha.)(9CI) (CA INDEX NAME)

L39 ANSWER 6 OF 6
ACCESSION NUMBER:
DOCUMENT NUMBER:
1995:45102 CAPLUS
122:188108
Peptidosteroidal Receptors for Opioid Peptides.
Sequence-Selective Binding Using a Synthetic Receptor
Library
Boyce, Rustum, Li, Ger, Nestler, H. Peter; Suenaga,
Toshiro; Still, W. Clark
Department of Chemistry, Columbia University, New
York, NY, 10027, USA
Journal of the American Chemical Society (1994),
116(17), 7955-6
CODEN: JACSAT; ISSN: 0002-7863
Journal

DOCUMENT TYPE:

116(17), 7955-6
CODEN: JACSAT; ISSN: 0002-7863

JOURNIT TYPE: JOURNAL

SUAGE: English

Peptidosteroids I (PS = polystyrene; VI = Ac-AA1-AA2-Gly and V2 =
Ac-AA3-AAA where AA = amino acid residues) were prepd. in 104 different
forms by encoded combinational chem. Using a series of enkephalin-like
opioid peptides as substrates, different substrates preferentially bind
different members of the above peptidosteroid receptor library.
161419-34-TOP, aminomethyl polystyrene resin-bound
161419-33-BDP, aminomethyl polystyrene resin-bound
161419-36-DDP, aminomethyl polystyrene resin-bound
161419-36-DDP, aminomethyl polystyrene resin-bound
161419-38-DDP, aminomethyl polystyrene resin-bound
161419-38-DDP, aminomethyl polystyrene resin-bound
161419-38-DDP, aminomethyl polystyrene resin-bound
RL: PEP (Physical, engineering or chemical process); SPN (Synthetic
preparation); PREC (Preparation); PRCC (Process)
(sequence-selective binding for opioid peptides using a synthetic
peptidosteroidal receptor library)
161419-34-7 CAPLUS
Cholan-24-oic acid, 3,7-dihydroxy-, 7-ester with N-[1-(N-acetyl-L-leucyl)L-prolyl]glycine, 3-ester with N-[N-(1-acetyl-L-prolyl)-Lphenylalanylglycine, (3.alpha.,5.beta.,7.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L39 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued)

PAGE 1-B

161419-36-9 CAPLUS
Cholan-24-oic acid, 3,7-dihydroxy-, 3-ester with N-[N-(N-acetyl-L-alanyl)-L-phenylalanyl]glycine, 7-ester with N-[1-(N-acetyl-L-valyl)-L-polyl]glycine, (3.alpha.,5.beta.,7.alpha.)- (9CI) (CA INDEX NAME)

L39 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2003 ACS

PAGE 1-B

L39 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2003 ACS

\_\_ CO2H

161419-37-0 CAPLUS Cholan-24-oic acid, 3,7-dihydroxy-, 3-ester with N-[N-(N2-acetyl-L-lysyl)-L-phenylalanyl]glycine, 7-ester with N-[N-(1-acetyl-L-prolyl)-L-phenylalanyl]glycine, (3.alpha.,5.beta.,7.alpha.) - (9CI) (CA INDEX NAME)

L39 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2003 ACS

PAGE 1-B

~pr-i

PAGE 1-B

\_\_ CO2H

161419-38-1 CAPLUS
Cholan-24-oic acid, 3,7-dihydroxy-, (3.fwdarw.1)-ester with
N-[N-(N-acetylglycyl)-L-.alpha.-aspartyl]glycine, 7-ester with
N-[N-(N-acetylglycyl)-L-valyl]glycine, (3.alpha.,5.beta.,7.alpha.)- (9CI)
(CA INDEX NAME)

=> d ibib ab hitstr 1-2

L38 ANSWER 1 OF 2 USPATFULL
ACCESSION NUMBER: 2002:172510 USPATFULL
TITLE: Steroid derived antibiotics
Savage, Paul B., Springville, UT, UNITED STATES
Li, Chunhong, Provo, UT, UNITED STATES

NUMBER KIND DATE

US 2002091278 A1 20020711
US 2001-930316 A1 20010815 (9)
Continuation-in-part of Ser. No. US 1999-234008, filed
on 19 Jan 1999, PATEMITED Continuation-in-part of Ser.
No. WO 1998-US4489, filed on 6 Mar 1998, UNXNOWN PATENT INFORMATION: APPLICATION INFO.: RELATED APPLN. INFO.:

NUMBER DATE

US 2000-225467P 20000815 (60)
Utility
APPLICATION
JOHN W. FREEMAN, ESO., Fish & Richardson P.C., 225
Franklin Street, Boston, MA, 02110-2804
58 PRIORITY INFORMATION: DOCUMENT TYPE: FILE SEGMENT: LEGAL REPRESENTATIVE:

LEGAL REPRESENTATIVE: JOHN W. FREEMAN, ESQ., Fish & Richardson P.C., 225
Franklin Street, Boston, MA, 02110-2804
NUMBER OF CLAIMS: 58
EXEMPLARY CLAIM: 1
NUMBER OF DRAWINGS: 10 Drawing Page(s)
LINE COUNT: 3770
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB A series of novel steroid derivatives are described. The steroid derivatives are antibacterial agents. The steroid derivatives also act to sensitize bacteria to other antibiotics including erythromyCin and novobiocin.

IT 302784-44-7 USPATFULL
CN Cholan-24-oic acid, 3,7,12-tris[(aminoacetyl)oxy]-,
(3.alpha.,5.beta.,7.alpha.,12.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

(prepn. o. 302784-51-6 f steroid derivs. as antibiotics) USPATFULL

L38 ANSWER 2 OF 2 USPATFULL ACCESSION NUMBER: 1998: TITLE: Synth

NTFULL
1998:108394 USPATFULL
Synthetic receptors, libraries and uses thereof
Still, W. Clark, Clinton, NY, United States
Li, Ge, Plainsboro, NJ, United States
The Trustees of Columbia University in The City of New
York, New York, NY, United States (U.S. corporation) INVENTOR(S):

PATENT ASSIGNEE(S):

NUMBER

ER KIND DATE US 5804563 1
US 1996-628972 1
Continuation of Ser. No. Jan 1994, now abandoned Utility Granted Hutzell, Paula K. Bakalyar, Heather A. Healin & Rothenberg, PC 14 19980908 19960408 (8) No. US 1994-181628, filed on 13 PATENT INFORMATION: APPLICATION INFO.: RELATED APPLN. INFO.: DOCUMENT TYPE:

FILE SEGMENT:
PRIMARY EXAMINER:
ASSISTANT EXAMINER:
LEGAL REPRESENTATIVE: NUMBER OF CLAIMS: EXEMPLARY CLAIM: NUMBER OF DRAWINGS:

6 Drawing Figure(s); 6 Drawing Page(s) 1877

LINE COUNT: 1877

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The invention is directed to synthetic receptor(s) which comprises a polyfunctional organic template covalently linked to two or more oligomers which may independently be the same or different and may independently be straight chain or branched. The template may be linked to an identifier which uniquely defines the synthetic receptor. The identifier is a stable chemical molecule or a plurality of stable chemical molecules distinguishable and detectable to picomolar levels or may be an oligonucleotide. In an preferred embodiment, the template is covalently linked to a solid support which is linked to an identifier.

IT 171762-33-7P

(Dreph. of synthetic receptors and libraries thereof)

171762-33-79
(prepn. of synthetic receptors and libraries thereof)
171762-37-7 USPATFULL
(Glycine, N-(N-acetyl-L-phenylalanyl)-, (3.alpha.,5.beta.,7.alpha.)-7[[(acetylamino)acetyl]oxy]-23-carboxy-24-norcholan-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry

L38 ANSWER 1 OF 2 USPATFULL (Continued)
CN Cholan-24-oic acid, 3,7,12-tris[[[(1,1-dimethylethoxy)carbonyl]amino]acet
yl]oxy]-, (3.alpha.,5.beta.,7.alpha.,12.alpha.)- (9CI) (CA INDEX NAME) Absolute stereochemistry, -

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10/930,316
         L39 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2002:522683 CAPLUS
137:79113
137:79113
137:7913
137:7913
137:7913
137:7913
137:7913
137:7913
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              DOCUMENT TYPE:
LANGUAGE:
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
US 2002091278 A1 20020711 US 2001-930316 20010815
WO 9944616 A1 19990910 WO 1998-US4489 19980306
W: AL, AM, AT, AU, AZ, BA, BE, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, LL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, XX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SS, LS, LT, JT, HT, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TH RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, GA, GN, ML, MR, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, GA, GN, ML, MR, NE, SN, TD, TO
US 6350738 B1 20020226 US 1999-234008 19990119
US 6350738 B1 20020226 US 1999-234008 19990119
US 0998-US4489 A2 19990119
US 2000-225467P P 20000815
OTHER SOURCE(S): MARPAT 137:79113
AB Novel steroid derivs. of formula I [R1-R4, R6, R7, R11, R12, R15-R17 - H, CH, alky1, hydroxyalky1, aminoalky1, aryl, etc.] are prepd. The steroid derivs. are antibacterial agents. The steroid derivs. also act to sensitize bacteria to other antibiotics including erythromycin and novobiocin. Thus, II was prepd. from My cholate. allyl bromide and benzylmethylamine in several steps. The prepd. compds. were tested against Gran-neg, bacteria.

17 302784-44-7 P
RL: PAC (Pharmacological activity): SFN (Synthetic preparation): THU (Therapeutic use): BIOL (Biological study): PREP (Preparation): USES (USB)
302784-44-7 CAPJUS
                                                        (Uses)
(prepn. of steroid derivs. as antibiotics)
302784-44-7 CAPUS
Cholan-24-oic acid, 3,7/12-tris[(aminoacetyl)oxy]-,
(3.alpha.,5.beta.,7.alpha.,12.alpha.)- (9CI) (CA INDEX NAME)
            Absolute stereochemistry.
            L39 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2003 ACS ACCESSION NUMBER: 2002:142730 CAPLUS DOCUMENT NUMBER: 136:200350
                                                                                                                                                                                                                                                     136:200350
Preparation of steroid derived antibiotics
Savage, Paul B.: Li, Chunchong
Brigham Young University, USA
PCT Int. Appl., 128 pp.
CODEN: PIXXD2
Patent
English
4
              INVENTOR(S):
              PATENT ASSIGNEE(S):
SOURCE:
              DOCUMENT TYPE:
LANGUAGE:
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FAMILY ACC. NUM. COUNT: PATENT INFORMATION: Absolute stereochemistry.

L39 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued)

RE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. of steroid derivs. as antibiotics) 302784-51-6 CAPLUS

Socretains Carlus Cholan-24-oic acid, 3,7,12-tris[[[[(1,1-dimethylethoxy)carbonyl]amino]acet yl]oxy]-, (3.alpha.,5.beta.,7.alpha.,12.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L39 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2003 ACS, (Continued)

302784-51-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
[prepn. of steroidal antibiotics)
302784-51-6 CaPLUS
Cholan-24-oic acid, 3,7,12-tris[[[[{1,1-dimethylethoxy)carbony1]amino]acet
yl]oxy]-, (3.alpha.,5.beta.,7.alpha.,12.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT:

THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT